Full wwPDB EM Validation Report

Nov 29, 2022 – 11:38 AM EST

PDB ID	:	8CYB
EMDB ID	:	EMD-27073
Title	:	SARS-CoV-2 Spike protein in complex with a pan-sarbecovirus nanobody 1-8
Authors	:	Huang, W.; Taylor, D.
Deposited on	:	2022-05-23
Resolution	:	2.70 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:

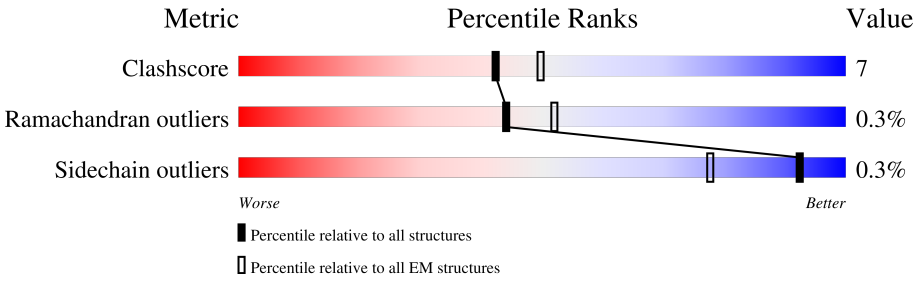
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	1273	75% 11% 13%
1	B	1273	75% 11% 13%
1	C	1273	77% 10% 13%
2	D	127	18% 85% 14%
3	E	2	100%
3	K	2	50% 50%
3	S	2	50% 50%
3	T	2	100%

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Mol	Chain	Length	Quality of chain
4	F	5	60% 40%
4	G	5	20% 60% 20%
4	H	5	80% 20%
4	J	5	20% 60% 20%
4	M	5	20% 40% 40%
4	O	5	80% 20%
4	V	5	20% 60% 20%
5	I	6	33% 33% 33%
6	L	3	33% 67%
6	P	3	67% 33%
6	Q	3	100%
6	R	3	67% 33%
6	U	3	100%
6	Y	3	67% 33%
6	Z	3	33% 33% 33%
7	N	4	25% 75%
8	W	4	50% 50%
9	X	3	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	H	1	-	-	X	-
4	BMA	M	3	-	-	X	-
6	NAG	R	1	-	-	X	-
7	NAG	N	2	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 54126 atoms, of which 25897 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	1102	Total	C	H	N	O	S	0	0
			16912	5471	8326	1435	1641	39		
1	B	1102	Total	C	H	N	O	S	0	0
			16923	5473	8333	1436	1642	39		
1	C	1102	Total	C	H	N	O	S	0	0
			16900	5471	8313	1436	1641	39		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called pan-sarbecovirus nanobody 1-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	126	Total	C	H	N	O	S	0	0
			1913	615	925	172	197	4		

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

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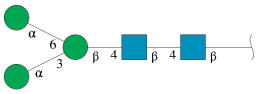
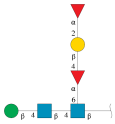
Mol	Chain	Residues	Atoms	AltConf	Trace
3	K	2	Total C N O 28 16 2 10	0	0
3	S	2	Total C N O 28 16 2 10	0	0
3	T	2	Total C N O 28 16 2 10	0	0

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



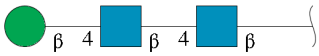
Mol	Chain	Residues	Atoms	AltConf	Trace
4	F	5	Total C N O 61 34 2 25	0	0
4	G	5	Total C N O 61 34 2 25	0	0
4	H	5	Total C N O 61 34 2 25	0	0
4	J	5	Total C N O 61 34 2 25	0	0
4	M	5	Total C N O 61 34 2 25	0	0
4	O	5	Total C N O 61 34 2 25	0	0
4	V	5	Total C N O 61 34 2 25	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-alpha-L-fucopyranose-(1-6)-[beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



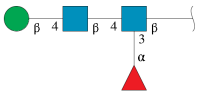
Mol	Chain	Residues	Atoms	AltConf	Trace
5	I	6	Total C N O 70 40 2 28	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	3	Total	C	N	O	0	0
			39	22	2	15		
6	P	3	Total	C	N	O	0	0
			39	22	2	15		
6	Q	3	Total	C	N	O	0	0
			39	22	2	15		
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	U	3	Total	C	N	O	0	0
			39	22	2	15		
6	Y	3	Total	C	N	O	0	0
			39	22	2	15		
6	Z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.

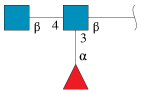


Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

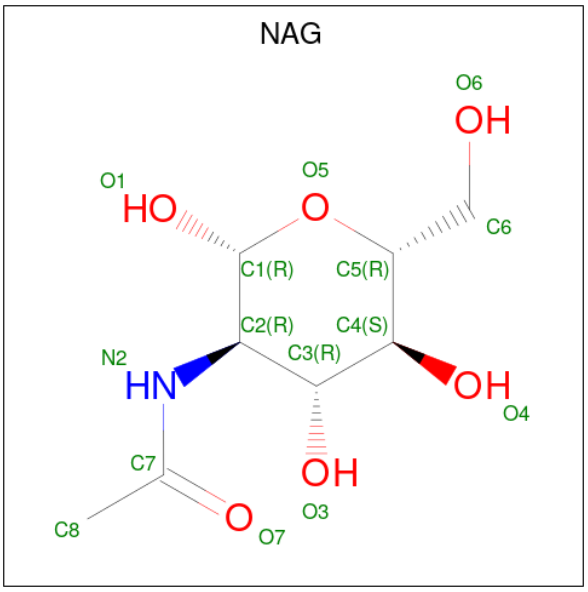
Mol	Chain	Residues	Atoms				AltConf	Trace
8	W	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C N O 154 88 11 55	0
10	A	1	Total C N O 154 88 11 55	0
10	A	1	Total C N O 154 88 11 55	0
10	A	1	Total C N O 154 88 11 55	0
10	A	1	Total C N O 154 88 11 55	0
10	A	1	Total C N O 154 88 11 55	0
10	A	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	B	1	Total C N O 154 88 11 55	0
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0

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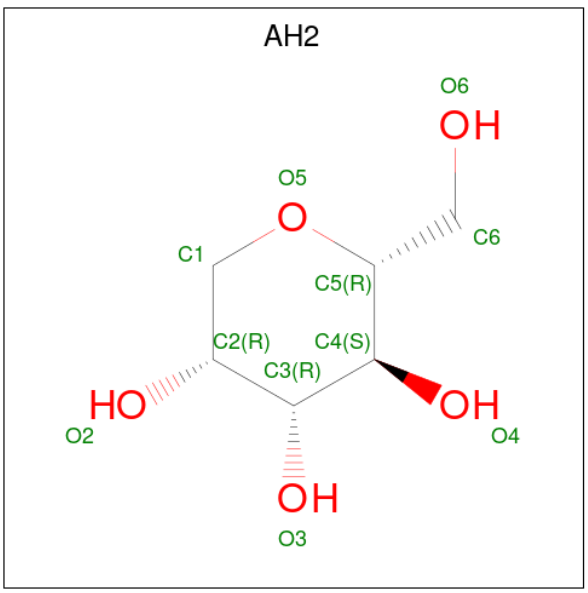
Mol	Chain	Residues	Atoms	AltConf
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0
10	C	1	Total C N O 140 80 10 50	0

- Molecule 11 is 1-deoxy-alpha-D-mannopyranose (three-letter code: AH2) (formula: $C_6H_{12}O_5$).



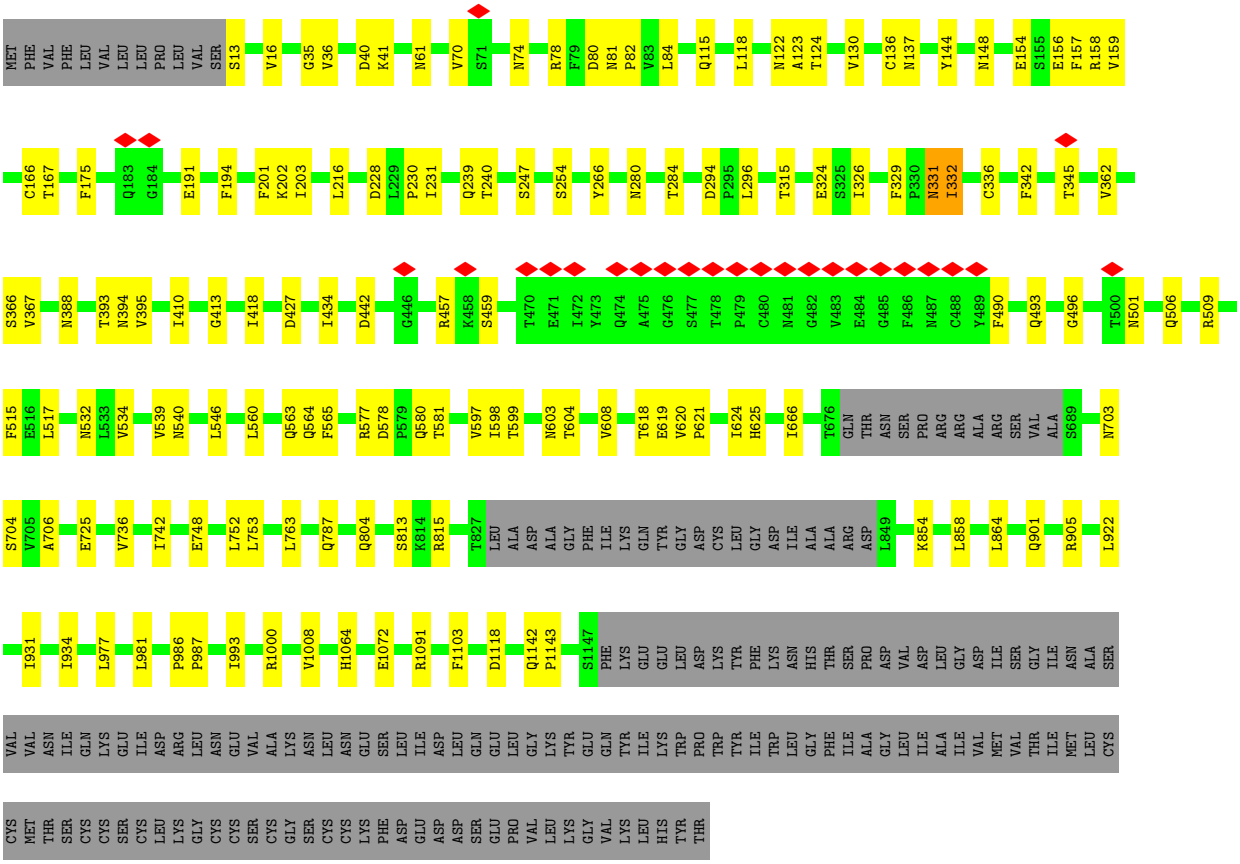
Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C O 11 6 5	0

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.

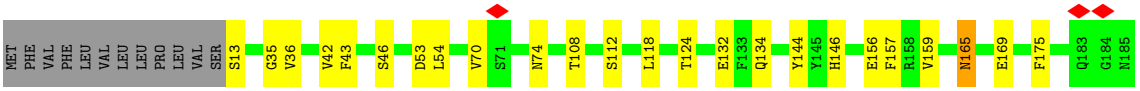
• Molecule 1: Spike glycoprotein

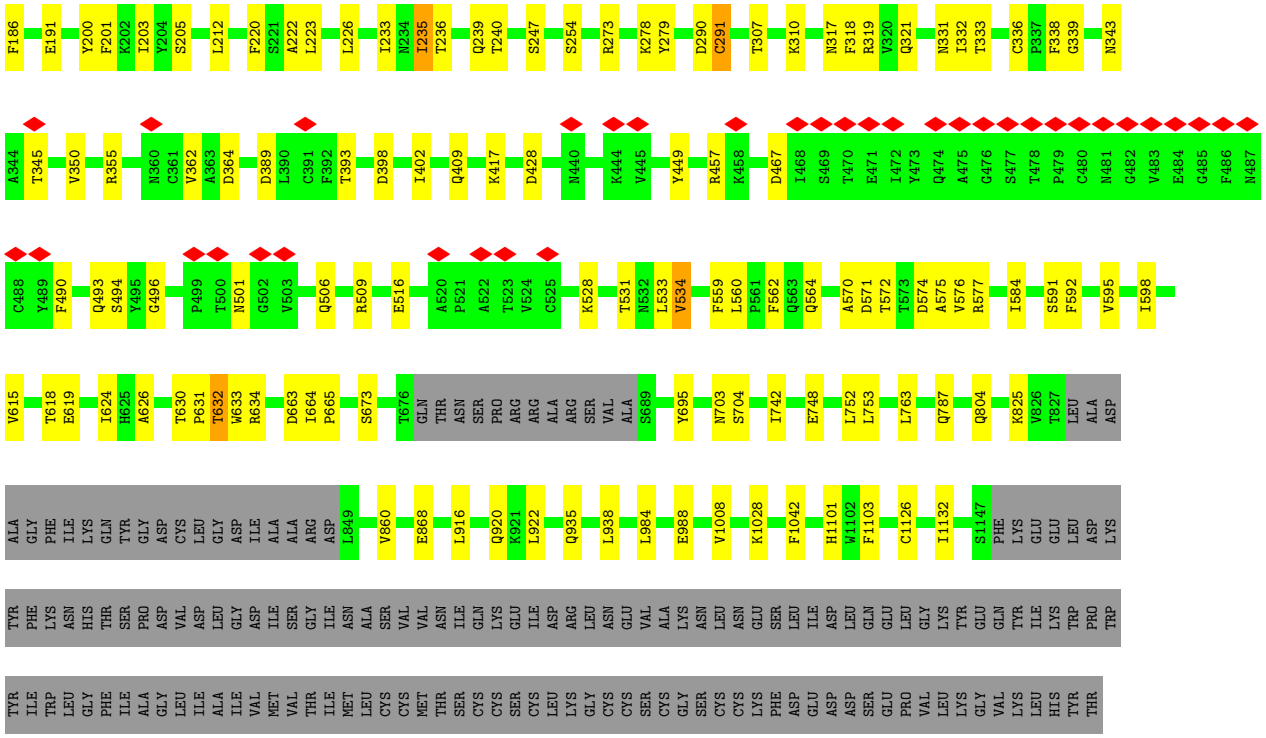
Chain A:



• Molecule 1: Spike glycoprotein

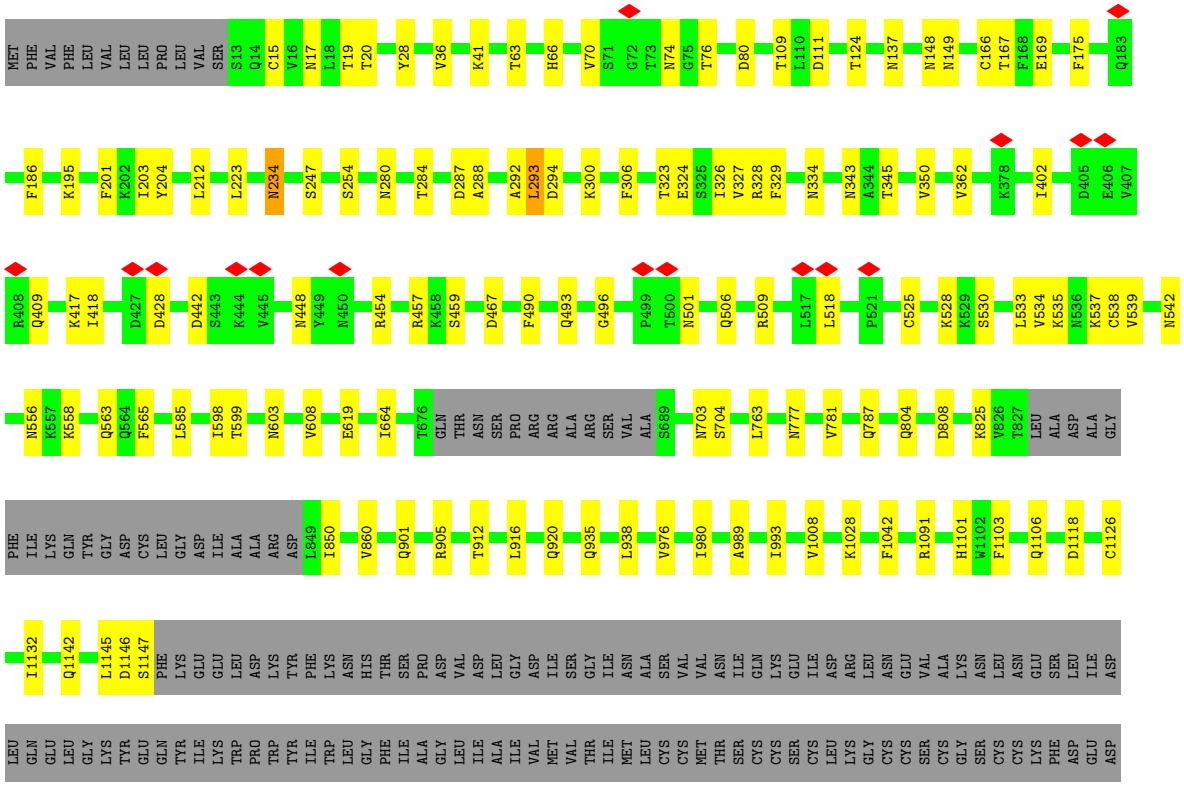
Chain B:

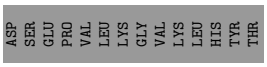




• Molecule 1: Spike glycoprotein

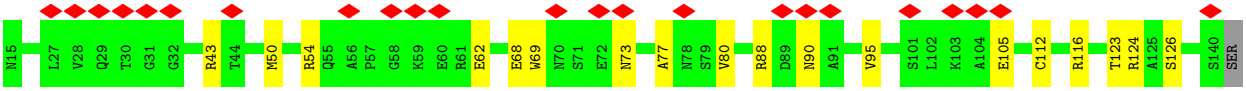
Chain C:





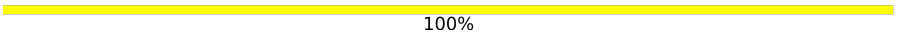
• Molecule 2: pan-sarbecovirus nanobody 1-8

Chain D:



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

Chain E:



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

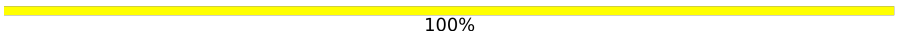
Chain K:

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

Chain S:

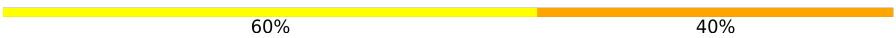
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



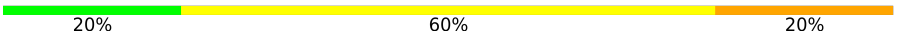
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



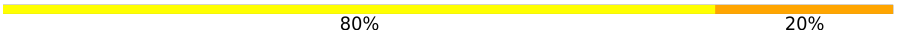
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



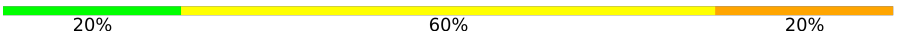
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



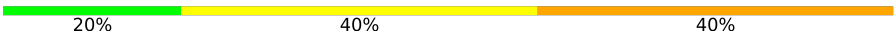
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



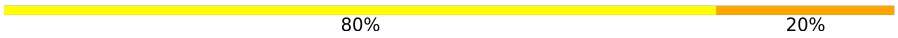
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



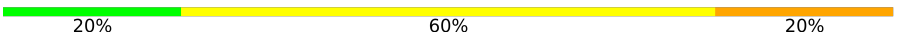
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

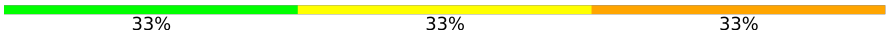


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

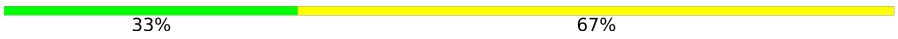
Chain V:



• Molecule 5: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-alpha-L-fucopyranose-(1-6)-[beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

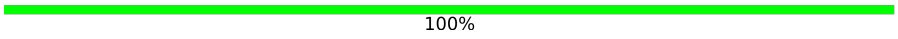
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

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

Chain P: 

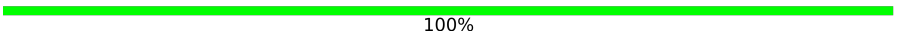
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 

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

Chain R: 

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

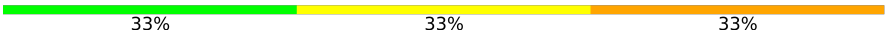
Chain U: 

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

Chain Y:

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

Chain Z:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

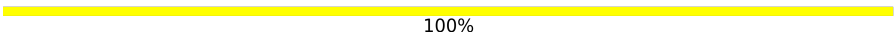
Chain N:

• Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 9: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4210888	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 ($e^-/Å^2$)	31.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.051	Depositor
Minimum map value	-0.770	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	425.28, 425.28, 425.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.329, 1.329, 1.329	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, GAL, AH2, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/8789	0.46	0/11972
1	B	0.24	0/8793	0.46	0/11977
1	C	0.25	0/8790	0.46	0/11972
2	D	0.24	0/1009	0.49	0/1365
All	All	0.25	0/27381	0.46	0/37286

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	149	ASN	Peptide

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	8586	8326	8331	103	0
1	B	8590	8333	8339	97	0
1	C	8587	8313	8335	93	0
2	D	988	925	925	12	0
3	E	28	0	25	2	0
3	K	28	0	25	4	0
3	S	28	0	25	8	0
3	T	28	0	25	1	0
4	F	61	0	52	9	0
4	G	61	0	52	2	0
4	H	61	0	52	14	0
4	J	61	0	52	2	0
4	M	61	0	52	10	0
4	O	61	0	52	6	0
4	V	61	0	52	3	0
5	I	70	0	61	6	0
6	L	39	0	34	1	0
6	P	39	0	34	1	0
6	Q	39	0	34	0	0
6	R	39	0	34	11	0
6	U	39	0	34	0	0
6	Y	39	0	34	3	0
6	Z	39	0	34	4	0
7	N	49	0	43	7	0
8	W	50	0	43	3	0
9	X	38	0	34	6	0
10	A	154	0	143	8	0
10	B	154	0	143	14	0
10	C	140	0	130	11	0
11	A	11	0	0	0	0
All	All	28229	25897	27229	399	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 7.

All (399) 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)
4:M:3:BMA:H4	4:M:4:MAN:H5	1.39	1.05
9:X:2:FUC:H3	9:X:3:NAG:H83	1.49	0.95
10:B:1311:NAG:H3	10:B:1311:NAG:H83	1.55	0.88
4:H:1:NAG:H83	4:H:1:NAG:H3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:1:NAG:H83	6:R:1:NAG:H3	1.56	0.87
3:S:1:NAG:H3	3:S:1:NAG:H83	1.55	0.87
3:K:2:NAG:H3	3:K:2:NAG:H83	1.56	0.87
10:B:1305:NAG:H3	10:B:1305:NAG:H83	1.55	0.87
7:N:2:NAG:H83	7:N:2:NAG:H3	1.54	0.87
4:F:1:NAG:H83	4:F:1:NAG:H3	1.55	0.84
4:M:3:BMA:H4	4:M:4:MAN:C5	2.07	0.84
10:B:1303:NAG:O7	10:B:1303:NAG:O4	1.97	0.83
1:C:901:GLN:OE1	1:C:905:ARG:NH1	2.12	0.83
4:O:2:NAG:HO3	4:O:3:BMA:HO2	1.16	0.83
1:B:626:ALA:O	1:B:634:ARG:NH2	2.11	0.83
1:A:239:GLN:NE2	1:A:240:THR:O	2.12	0.83
10:C:1304:NAG:H83	10:C:1304:NAG:H3	1.61	0.82
4:M:3:BMA:O2	4:M:4:MAN:O5	1.97	0.82
1:A:427:ASP:O	2:D:116:ARG:NH2	2.12	0.81
1:C:234:ASN:OD1	1:C:234:ASN:N	2.14	0.81
1:C:329:PHE:CG	1:C:528:LYS:HE3	2.17	0.80
4:F:3:BMA:O2	4:F:4:MAN:O5	2.00	0.80
1:C:534:VAL:HG11	1:C:539:VAL:HG11	1.62	0.79
4:H:2:NAG:O4	4:H:2:NAG:O7	2.02	0.77
1:B:336:CYS:N	1:B:362:VAL:O	2.17	0.77
4:H:3:BMA:H3	4:H:4:MAN:H5	1.65	0.77
1:B:124:THR:O	1:B:175:PHE:N	2.18	0.76
9:X:1:NAG:H61	9:X:3:NAG:O5	1.86	0.76
1:B:496:GLY:O	1:B:501:ASN:ND2	2.19	0.75
1:A:324:GLU:N	1:A:324:GLU:OE1	2.19	0.75
1:B:132:GLU:OE2	10:B:1307:NAG:N2	2.19	0.75
1:C:169:GLU:OE1	1:C:169:GLU:N	2.20	0.75
1:A:496:GLY:O	1:A:501:ASN:ND2	2.21	0.74
1:A:578:ASP:OD2	1:A:581:THR:OG1	2.05	0.74
1:B:239:GLN:NE2	1:B:240:THR:O	2.22	0.73
1:B:319:ARG:NH1	1:B:321:GLN:OE1	2.20	0.73
1:A:124:THR:O	1:A:175:PHE:N	2.21	0.73
1:A:247:SER:OG	1:A:254:SER:O	2.06	0.73
1:B:112:SER:OG	1:B:134:GLN:OE1	2.04	0.73
1:B:618:THR:OG1	1:B:619:GLU:OE1	2.06	0.72
3:S:2:NAG:O6	3:S:2:NAG:O3	2.06	0.72
1:B:570:ALA:O	1:B:572:THR:HG23	1.90	0.71
1:C:195:LYS:NZ	1:C:204:TYR:OH	2.23	0.71
1:C:490:PHE:O	1:C:493:GLN:NE2	2.23	0.71
1:C:324:GLU:OE1	1:C:324:GLU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:TRP:O	2:D:88:ARG:NH1	2.24	0.71
1:C:124:THR:O	1:C:175:PHE:N	2.23	0.71
1:C:247:SER:OG	1:C:254:SER:O	2.07	0.71
1:A:118:LEU:HD11	1:A:159:VAL:HG11	1.72	0.70
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.24	0.70
1:A:490:PHE:O	1:A:493:GLN:NE2	2.24	0.70
4:H:3:BMA:H3	4:H:4:MAN:H3	1.73	0.70
1:C:533:LEU:O	1:C:533:LEU:HD23	1.93	0.69
5:I:5:NAG:H5	5:I:6:BMA:O2	1.93	0.69
1:A:331:ASN:O	1:A:332:ILE:HG22	1.93	0.68
1:C:201:PHE:HE1	1:C:203:ILE:HD11	1.59	0.68
1:C:525:CYS:CB	1:C:528:LYS:HD2	2.22	0.68
1:B:825:LYS:NZ	1:B:938:LEU:O	2.26	0.68
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.28	0.67
1:B:144:TYR:OH	1:B:156:GLU:OE2	2.08	0.67
1:C:777:ASN:O	1:C:781:VAL:HG23	1.95	0.67
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.77	0.67
6:Z:2:NAG:H5	6:Z:3:BMA:O2	1.95	0.67
4:M:3:BMA:HO2	4:M:4:MAN:C1	2.07	0.67
3:S:2:NAG:HO3	3:S:2:NAG:HO6	1.40	0.67
1:A:563:GLN:O	1:A:577:ARG:NH1	2.28	0.67
1:B:236:THR:HG21	10:B:1306:NAG:H81	1.76	0.67
6:Z:2:NAG:H3	6:Z:3:BMA:O2	1.95	0.66
1:A:144:TYR:OH	1:A:156:GLU:OE2	2.05	0.66
1:A:413:GLY:O	2:D:43:ARG:NH1	2.29	0.66
1:C:457:ARG:NH1	1:C:459:SER:O	2.28	0.66
1:B:339:GLY:O	1:B:343:ASN:N	2.28	0.65
1:C:326:ILE:HD12	1:C:534:VAL:HG12	1.78	0.65
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.77	0.65
1:B:169:GLU:N	1:B:169:GLU:OE1	2.28	0.65
1:B:247:SER:OG	1:B:254:SER:O	2.12	0.65
5:I:5:NAG:H3	5:I:6:BMA:O2	1.96	0.65
1:A:201:PHE:CE1	1:A:203:ILE:HD11	2.31	0.65
7:N:2:NAG:C7	7:N:4:FUC:H5	2.27	0.65
9:X:2:FUC:H3	9:X:3:NAG:C8	2.25	0.65
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.30	0.64
1:C:201:PHE:CE1	1:C:203:ILE:HD11	2.33	0.64
4:H:3:BMA:H3	4:H:4:MAN:C5	2.27	0.64
1:B:490:PHE:O	1:B:493:GLN:NE2	2.31	0.63
2:D:50:MET:HG2	2:D:95:VAL:HG21	1.81	0.63
1:C:148:ASN:HD22	10:C:1304:NAG:H81	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:1:NAG:O4	3:S:2:NAG:O6	2.12	0.63
1:C:300:LYS:NZ	1:C:306:PHE:O	2.25	0.63
1:A:136:CYS:HB3	10:A:1301:NAG:H83	1.79	0.63
3:S:1:NAG:H83	3:S:2:NAG:H83	1.81	0.63
1:A:563:GLN:O	1:A:564:GLN:NE2	2.32	0.62
1:A:618:THR:OG1	1:A:619:GLU:OE1	2.07	0.62
6:R:1:NAG:H61	6:R:2:NAG:N2	2.14	0.62
1:A:70:VAL:HG11	1:A:74:ASN:HB2	1.82	0.62
1:B:1103:PHE:HZ	4:M:1:NAG:H62	1.65	0.61
6:R:2:NAG:O3	6:R:3:BMA:O5	2.18	0.61
1:A:598:ILE:HD13	1:A:666:ILE:HD12	1.82	0.61
1:B:393:THR:OG1	1:B:516:GLU:O	2.17	0.61
1:C:496:GLY:O	1:C:501:ASN:ND2	2.33	0.61
1:C:329:PHE:CD2	1:C:528:LYS:HE3	2.35	0.60
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.34	0.60
10:B:1311:NAG:H3	10:B:1311:NAG:C8	2.31	0.60
1:A:442:ASP:OD2	1:A:509:ARG:NE	2.34	0.60
1:C:137:ASN:ND2	10:C:1301:NAG:H62	2.17	0.60
4:F:3:BMA:O4	4:F:4:MAN:H2	2.01	0.60
1:C:825:LYS:NZ	1:C:938:LEU:O	2.29	0.59
1:A:148:ASN:HB3	10:A:1304:NAG:H82	1.85	0.59
10:C:1304:NAG:H83	10:C:1304:NAG:C3	2.32	0.59
1:A:336:CYS:N	1:A:362:VAL:O	2.35	0.59
1:C:28:TYR:CE1	1:C:63:THR:HG22	2.38	0.59
4:H:3:BMA:H3	4:H:4:MAN:C3	2.33	0.59
1:A:81:ASN:OD1	1:A:239:GLN:NE2	2.36	0.58
1:A:532:ASN:OD1	1:A:580:GLN:NE2	2.36	0.58
1:B:787:GLN:OE1	1:C:703:ASN:ND2	2.36	0.58
1:B:70:VAL:HG11	1:B:74:ASN:HB2	1.86	0.58
1:A:706:ALA:CB	5:I:1:NAG:H61	2.34	0.58
1:B:42:VAL:O	1:C:563:GLN:NE2	2.35	0.58
1:A:326:ILE:HD12	1:A:534:VAL:HB	1.84	0.58
3:S:1:NAG:H3	3:S:1:NAG:C8	2.31	0.58
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.38	0.58
1:B:703:ASN:OD1	1:B:704:SER:N	2.36	0.58
1:A:367:VAL:HG11	10:A:1308:NAG:H62	1.86	0.57
3:E:1:NAG:O3	3:E:2:NAG:O5	2.20	0.57
1:B:201:PHE:HD2	1:B:203:ILE:HD11	1.68	0.57
1:C:234:ASN:HB2	10:C:1306:NAG:H2	1.85	0.57
1:A:326:ILE:HG13	1:A:539:VAL:HG11	1.85	0.57
1:C:70:VAL:HG11	1:C:74:ASN:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:HG21	1:A:597:VAL:HG23	1.85	0.57
1:C:343:ASN:HA	10:C:1308:NAG:H2	1.86	0.57
9:X:1:NAG:H4	9:X:3:NAG:N2	2.14	0.57
4:H:1:NAG:H3	4:H:1:NAG:C8	2.31	0.57
1:B:290:ASP:OD1	1:B:291:CYS:N	2.38	0.56
1:B:632:THR:OG1	1:B:633:TRP:N	2.38	0.56
1:C:525:CYS:HB3	1:C:528:LYS:HD2	1.86	0.56
6:R:1:NAG:H3	6:R:1:NAG:C8	2.32	0.56
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.87	0.56
7:N:2:NAG:H3	7:N:2:NAG:C8	2.30	0.56
1:C:36:VAL:O	1:C:223:LEU:N	2.33	0.56
4:F:1:NAG:H3	4:F:1:NAG:C8	2.31	0.56
1:A:1091:ARG:NH1	1:A:1118:ASP:OD1	2.38	0.56
1:A:393:THR:HG23	1:A:517:LEU:HD12	1.88	0.56
1:C:15:CYS:O	10:C:1301:NAG:H82	2.06	0.55
1:B:1101:HIS:ND1	4:M:1:NAG:H5	2.20	0.55
10:B:1305:NAG:H3	10:B:1305:NAG:C8	2.31	0.55
1:C:556:ASN:O	1:C:558:LYS:NZ	2.40	0.55
1:C:850:ILE:HG23	1:C:860:VAL:HG21	1.88	0.55
1:B:916:LEU:O	1:B:920:GLN:N	2.39	0.55
1:C:501:ASN:O	1:C:506:GLN:NE2	2.39	0.55
1:C:442:ASP:O	1:C:448:ASN:ND2	2.39	0.54
1:C:1103:PHE:HZ	6:Y:1:NAG:H62	1.72	0.54
1:A:501:ASN:O	1:A:506:GLN:NE2	2.41	0.54
1:B:53:ASP:OD1	1:B:54:LEU:N	2.36	0.54
1:A:230:PRO:O	1:A:231:ILE:HD13	2.08	0.54
2:D:54:ARG:NE	2:D:62:GLU:OE1	2.40	0.54
4:H:1:NAG:H61	4:H:2:NAG:O5	2.07	0.54
4:O:3:BMA:H4	4:O:5:MAN:H3	1.88	0.54
1:C:535:LYS:NZ	1:C:585:LEU:HD22	2.22	0.54
1:A:13:SER:N	1:A:157:PHE:O	2.40	0.54
1:B:624:ILE:HG23	1:B:626:ALA:H	1.73	0.54
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.90	0.54
1:C:703:ASN:OD1	1:C:704:SER:N	2.41	0.54
1:A:201:PHE:CD1	1:A:203:ILE:HD11	2.44	0.53
1:B:205:SER:H	1:B:226:LEU:HD23	1.74	0.53
3:S:1:NAG:H82	3:S:1:NAG:C1	2.39	0.53
5:I:5:NAG:H5	5:I:6:BMA:C2	2.39	0.53
1:A:813:SER:OG	1:A:815:ARG:NH1	2.41	0.53
1:C:329:PHE:CE2	1:C:528:LYS:HG2	2.43	0.53
3:K:2:NAG:H3	3:K:2:NAG:C8	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:1:NAG:H4	6:R:2:NAG:C7	2.38	0.53
1:A:804:GLN:NE2	4:H:1:NAG:H62	2.23	0.53
4:F:1:NAG:C1	4:F:1:NAG:H82	2.39	0.53
1:B:868:GLU:N	1:B:868:GLU:OE1	2.41	0.53
10:B:1311:NAG:C1	10:B:1311:NAG:H82	2.39	0.53
1:B:201:PHE:CD2	1:B:203:ILE:HD11	2.44	0.53
3:K:2:NAG:H82	3:K:2:NAG:C1	2.39	0.53
4:H:1:NAG:C1	4:H:1:NAG:H82	2.39	0.53
1:A:154:GLU:OE1	10:A:1303:NAG:O6	2.15	0.52
1:A:599:THR:HB	1:A:608:VAL:HG12	1.91	0.52
1:A:977:LEU:HD22	1:A:993:ILE:HD12	1.92	0.52
10:A:1308:NAG:O7	10:A:1308:NAG:O3	2.25	0.52
6:R:1:NAG:H61	6:R:2:NAG:HN2	1.73	0.52
4:V:3:BMA:H4	4:V:5:MAN:O5	2.09	0.52
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.42	0.52
6:R:1:NAG:C1	6:R:1:NAG:H82	2.39	0.52
1:B:205:SER:N	1:B:226:LEU:HD23	2.24	0.52
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.75	0.52
10:B:1305:NAG:C1	10:B:1305:NAG:H82	2.39	0.52
4:F:3:BMA:H4	4:F:4:MAN:O5	2.09	0.52
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.43	0.52
1:B:36:VAL:O	1:B:223:LEU:N	2.41	0.52
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.91	0.52
1:B:118:LEU:HD11	1:B:159:VAL:HG11	1.91	0.51
7:N:2:NAG:H82	7:N:2:NAG:C1	2.39	0.51
1:A:410:ILE:HD11	1:A:418:ILE:CG2	2.40	0.51
1:B:501:ASN:O	1:B:506:GLN:NE2	2.43	0.51
1:C:350:VAL:HG23	1:C:402:ILE:HG22	1.92	0.51
1:A:410:ILE:HD11	1:A:418:ILE:HG21	1.93	0.51
1:A:619:GLU:OE1	1:A:619:GLU:N	2.43	0.51
1:B:1103:PHE:CZ	4:M:1:NAG:H62	2.44	0.51
1:A:703:ASN:ND2	1:C:787:GLN:OE1	2.44	0.51
1:B:355:ARG:NE	1:B:398:ASP:OD1	2.37	0.51
1:B:560:LEU:HD23	1:B:562:PHE:CE2	2.45	0.51
1:B:860:VAL:HG13	1:B:860:VAL:O	2.11	0.51
1:A:922:LEU:CD1	4:G:2:NAG:H82	2.41	0.51
1:A:580:GLN:O	3:E:1:NAG:H82	2.11	0.51
1:A:166:CYS:SG	1:A:167:THR:N	2.84	0.50
1:B:449:TYR:O	1:B:494:SER:OG	2.28	0.50
1:B:233:ILE:HG23	1:B:235:ILE:HG13	1.94	0.50
1:A:1103:PHE:HZ	4:J:1:NAG:H62	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.40	0.49
1:A:326:ILE:CG1	1:A:539:VAL:HG11	2.42	0.49
1:B:200:TYR:CE2	1:C:518:LEU:HD22	2.47	0.49
1:C:343:ASN:CA	10:C:1308:NAG:H2	2.42	0.49
1:B:631:PRO:O	1:B:632:THR:OG1	2.23	0.49
1:B:273:ARG:NH2	1:B:291:CYS:O	2.43	0.49
1:B:984:LEU:HD12	1:B:988:GLU:HG3	1.94	0.49
6:R:1:NAG:O6	6:R:2:NAG:H83	2.12	0.49
1:B:290:ASP:O	1:B:291:CYS:CB	2.61	0.49
1:B:531:THR:HG23	1:B:531:THR:O	2.13	0.49
1:C:287:ASP:OD1	1:C:288:ALA:N	2.45	0.49
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.45	0.49
1:B:570:ALA:O	1:B:571:ASP:OD1	2.30	0.49
1:C:334:ASN:O	1:C:362:VAL:N	2.37	0.48
3:T:1:NAG:H3	3:T:2:NAG:C7	2.43	0.48
1:A:394:ASN:OD1	1:A:395:VAL:N	2.46	0.48
1:C:534:VAL:HG22	1:C:537:LYS:HB3	1.95	0.48
2:D:50:MET:CE	2:D:112:CYS:HB2	2.42	0.48
8:W:2:NAG:H61	8:W:3:BMA:C1	2.43	0.48
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.95	0.48
1:B:1101:HIS:CG	4:M:1:NAG:H5	2.48	0.48
1:C:535:LYS:HZ3	1:C:585:LEU:HD22	1.78	0.48
1:A:787:GLN:OE1	1:A:787:GLN:N	2.46	0.48
4:V:3:BMA:O2	4:V:5:MAN:H62	2.13	0.48
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.29	0.47
1:A:986:PRO:N	1:A:987:PRO:HD2	2.28	0.47
10:C:1304:NAG:C1	10:C:1304:NAG:H82	2.45	0.47
4:F:3:BMA:H5	4:F:5:MAN:C5	2.44	0.47
1:A:137:ASN:HB2	10:A:1301:NAG:H3	1.95	0.47
1:C:329:PHE:CD2	1:C:528:LYS:HG2	2.50	0.47
4:F:1:NAG:H61	4:F:2:NAG:C7	2.45	0.47
1:B:307:THR:HG23	1:B:307:THR:O	2.13	0.47
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.12	0.47
1:A:736:VAL:HG13	1:A:858:LEU:HD23	1.97	0.47
1:C:166:CYS:SG	1:C:167:THR:N	2.88	0.47
4:M:3:BMA:H4	4:M:4:MAN:H3	1.97	0.47
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.48	0.46
10:C:1304:NAG:C3	10:C:1304:NAG:C8	2.91	0.46
8:W:1:NAG:H62	8:W:2:NAG:H82	1.97	0.46
1:B:200:TYR:HE2	1:C:518:LEU:HD22	1.80	0.46
1:C:186:PHE:N	1:C:212:LEU:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:GLU:OE1	1:B:619:GLU:N	2.47	0.46
6:Z:2:NAG:H5	6:Z:3:BMA:C2	2.45	0.46
1:A:118:LEU:CD1	1:A:159:VAL:HG11	2.44	0.46
1:B:332:ILE:HG23	1:B:333:THR:N	2.31	0.46
1:A:901:GLN:OE1	1:A:905:ARG:NH1	2.48	0.46
7:N:1:NAG:H4	7:N:2:NAG:H2	1.44	0.46
1:C:1146:ASP:OD1	1:C:1147:SER:N	2.48	0.46
2:D:105:GLU:OE1	2:D:105:GLU:N	2.48	0.46
4:V:2:NAG:O3	4:V:3:BMA:H2	2.15	0.46
6:Z:2:NAG:C3	6:Z:3:BMA:O5	2.64	0.46
1:B:922:LEU:CD1	6:P:2:NAG:H83	2.46	0.45
1:C:538:CYS:O	1:C:539:VAL:HG13	2.17	0.45
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.45	0.45
1:A:194:PHE:CE1	1:A:203:ILE:HG23	2.52	0.45
1:A:864:LEU:HD11	1:B:665:PRO:HB3	1.97	0.45
2:D:88:ARG:NH1	2:D:90:ASN:OD1	2.50	0.45
1:A:560:LEU:HD12	1:C:41:LYS:HE2	1.98	0.45
1:A:977:LEU:O	1:A:981:LEU:HD23	2.17	0.45
4:H:1:NAG:H4	4:H:2:NAG:H2	1.73	0.45
1:A:345:THR:O	1:A:509:ARG:NH2	2.49	0.45
1:B:457:ARG:NE	1:B:467:ASP:OD2	2.32	0.45
8:W:3:BMA:H4	8:W:4:MAN:O5	2.16	0.45
1:A:332:ILE:HD11	1:A:362:VAL:HG11	1.99	0.45
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.39	0.45
1:C:327:VAL:HG22	1:C:542:ASN:HB3	1.98	0.45
4:O:2:NAG:O3	4:O:3:BMA:O2	2.05	0.45
1:C:292:ALA:O	1:C:293:LEU:C	2.55	0.45
1:C:850:ILE:CG2	1:C:860:VAL:HG21	2.46	0.45
1:A:457:ARG:NH1	1:A:459:SER:O	2.46	0.44
1:B:574:ASP:OD1	1:B:575:ALA:N	2.51	0.44
1:A:122:ASN:O	1:A:123:ALA:HB3	2.17	0.44
1:B:673:SER:OG	1:B:695:TYR:OH	2.35	0.44
1:C:1103:PHE:CZ	6:Y:1:NAG:H62	2.50	0.44
1:A:599:THR:CB	1:A:608:VAL:HG12	2.47	0.44
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.98	0.44
1:A:35:GLY:O	1:A:36:VAL:HG23	2.18	0.44
1:B:332:ILE:HD11	1:B:362:VAL:HG12	2.00	0.44
1:B:389:ASP:OD2	1:B:528:LYS:NZ	2.30	0.44
1:C:454:ARG:NH2	1:C:467:ASP:O	2.46	0.44
1:A:748:GLU:O	1:A:752:LEU:HD13	2.17	0.44
1:B:36:VAL:HG23	1:B:222:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:VAL:HG23	1:B:402:ILE:HG22	2.00	0.44
1:C:442:ASP:OD2	1:C:509:ARG:NE	2.51	0.44
1:A:40:ASP:OD1	1:A:41:LYS:N	2.51	0.44
2:D:68:GLU:OE1	2:D:73:ASN:N	2.50	0.44
1:A:194:PHE:CD1	1:A:203:ILE:HG23	2.53	0.44
1:B:165:ASN:HD22	10:B:1307:NAG:H83	1.81	0.44
1:A:191:GLU:N	1:A:191:GLU:OE1	2.50	0.43
1:B:317:ASN:OD1	1:B:318:PHE:N	2.51	0.43
1:A:61:ASN:HB2	10:A:1302:NAG:H2	1.99	0.43
1:A:280:ASN:OD1	1:A:284:THR:N	2.47	0.43
1:A:620:VAL:HG12	1:A:621:PRO:HD3	2.00	0.43
1:B:345:THR:O	1:B:509:ARG:NH2	2.49	0.43
1:C:409:GLN:OE1	1:C:418:ILE:N	2.45	0.43
1:C:912:THR:HG23	1:C:1106:GLN:OE1	2.18	0.43
2:D:124:ARG:NE	2:D:126:SER:OG	2.45	0.43
1:A:78:ARG:NE	1:A:80:ASP:OD1	2.51	0.43
1:A:546:LEU:HD12	1:A:565:PHE:CD1	2.53	0.43
1:A:1142:GLN:HG3	1:A:1143:PRO:HD3	2.00	0.43
1:B:35:GLY:O	1:B:36:VAL:HG13	2.18	0.43
10:B:1308:NAG:O3	10:B:1308:NAG:H82	2.18	0.43
1:C:292:ALA:O	1:C:294:ASP:N	2.51	0.43
1:C:599:THR:HB	1:C:608:VAL:HG12	1.99	0.43
1:B:742:ILE:HG21	1:B:753:LEU:HD12	1.99	0.43
1:C:70:VAL:HG12	1:C:76:THR:H	1.84	0.43
1:C:619:GLU:N	1:C:619:GLU:OE1	2.50	0.43
1:A:624:ILE:O	1:A:625:HIS:ND1	2.51	0.43
1:B:191:GLU:HB2	1:B:223:LEU:HD11	2.01	0.43
1:B:332:ILE:HG12	1:B:364:ASP:OD1	2.18	0.43
1:C:327:VAL:HB	1:C:530:SER:OG	2.18	0.43
6:R:1:NAG:H83	6:R:1:NAG:C3	2.39	0.43
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.01	0.43
1:B:576:VAL:HG22	1:B:577:ARG:N	2.33	0.43
4:J:3:BMA:H62	4:J:5:MAN:H2	1.56	0.43
1:B:46:SER:N	1:B:279:TYR:O	2.51	0.43
1:B:630:THR:OG1	1:B:631:PRO:CD	2.67	0.43
1:B:13:SER:N	1:B:157:PHE:O	2.51	0.43
4:H:1:NAG:C8	4:H:1:NAG:C1	2.97	0.43
4:F:1:NAG:C8	4:F:1:NAG:C1	2.97	0.43
1:A:703:ASN:OD1	1:A:704:SER:N	2.52	0.43
4:G:3:BMA:H62	4:G:5:MAN:H2	1.31	0.42
3:K:2:NAG:C8	3:K:2:NAG:C1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:O	1:A:580:GLN:NE2	2.51	0.42
1:B:559:PHE:CE2	1:B:584:ILE:HG23	2.54	0.42
1:C:976:VAL:O	1:C:980:ILE:HD12	2.18	0.42
7:N:1:NAG:H61	7:N:2:NAG:O5	2.18	0.42
1:A:804:GLN:HE22	4:H:1:NAG:H62	1.84	0.42
10:B:1305:NAG:C8	10:B:1305:NAG:C1	2.97	0.42
10:B:1311:NAG:C8	10:B:1311:NAG:C1	2.97	0.42
1:C:428:ASP:OD1	1:C:428:ASP:N	2.52	0.42
5:I:5:NAG:C3	5:I:6:BMA:O5	2.67	0.42
1:B:336:CYS:O	1:B:338:PHE:N	2.47	0.42
1:C:980:ILE:HD12	1:C:980:ILE:H	1.84	0.42
6:R:1:NAG:C8	6:R:1:NAG:C1	2.97	0.42
3:S:1:NAG:C8	3:S:1:NAG:C1	2.97	0.42
1:A:82:PRO:HB2	1:A:84:LEU:HD12	2.01	0.42
1:A:342:PHE:HZ	1:A:434:ILE:HD12	1.85	0.42
2:D:123:THR:HG23	2:D:124:ARG:N	2.35	0.42
4:O:3:BMA:H62	4:O:5:MAN:H2	1.21	0.42
1:C:1142:GLN:HA	1:C:1145:LEU:HD13	2.02	0.42
5:I:1:NAG:H62	5:I:2:FUC:H2	1.60	0.42
1:A:539:VAL:HG22	1:A:540:ASN:N	2.35	0.42
1:A:620:VAL:N	1:A:621:PRO:CD	2.83	0.42
1:B:673:SER:HG	1:B:695:TYR:HE2	1.62	0.42
1:A:16:VAL:HG21	1:A:158:ARG:NH1	2.34	0.42
1:A:366:SER:OG	1:A:388:ASN:ND2	2.44	0.42
4:O:1:NAG:H62	4:O:2:NAG:C7	2.49	0.42
1:B:43:PHE:HD2	1:C:565:PHE:O	2.03	0.42
1:B:290:ASP:O	1:B:291:CYS:HB3	2.20	0.42
1:B:533:LEU:O	1:B:534:VAL:O	2.37	0.42
1:A:315:THR:HG21	1:A:597:VAL:CG2	2.49	0.41
1:B:146:HIS:CD2	10:B:1308:NAG:H83	2.55	0.41
1:B:186:PHE:N	1:B:212:LEU:O	2.47	0.41
1:C:808:ASP:OD1	1:C:808:ASP:N	2.48	0.41
2:D:77:ALA:HB3	2:D:80:VAL:HG22	2.02	0.41
9:X:1:NAG:H4	9:X:3:NAG:H2	1.55	0.41
1:B:748:GLU:O	1:B:752:LEU:HD13	2.19	0.41
6:L:1:NAG:H61	6:L:2:NAG:C7	2.51	0.41
4:M:3:BMA:H62	4:M:5:MAN:H2	1.26	0.41
1:A:854:LYS:HD2	1:A:854:LYS:O	2.21	0.41
1:C:66:HIS:N	1:C:80:ASP:OD2	2.53	0.41
1:C:327:VAL:HG13	1:C:542:ASN:HB3	2.02	0.41
1:C:345:THR:O	1:C:509:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLN:OE1	1:C:417:LYS:N	2.53	0.41
1:C:916:LEU:O	1:C:920:GLN:N	2.53	0.41
7:N:2:NAG:C8	7:N:2:NAG:C1	2.98	0.41
4:O:1:NAG:O3	4:O:1:NAG:H82	2.19	0.41
9:X:1:NAG:H61	9:X:3:NAG:C1	2.50	0.41
1:C:19:THR:OG1	1:C:20:THR:N	2.53	0.41
1:C:280:ASN:OD1	1:C:284:THR:N	2.50	0.41
1:C:328:ARG:CZ	1:C:533:LEU:HD12	2.50	0.41
1:A:115:GLN:HE22	10:A:1305:NAG:H62	1.85	0.41
1:B:564:GLN:O	1:B:577:ARG:N	2.53	0.41
4:H:3:BMA:C3	4:H:4:MAN:H5	2.44	0.41
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.86	0.41
1:A:81:ASN:N	1:A:82:PRO:HD3	2.36	0.41
1:A:604:THR:HG22	1:A:604:THR:O	2.21	0.41
1:C:1101:HIS:ND1	6:Y:1:NAG:H5	2.36	0.41
1:A:216:LEU:HD13	1:A:266:TYR:HE1	1.86	0.40
1:A:296:LEU:HB2	1:A:608:VAL:HG11	2.02	0.40
1:B:108:THR:HA	1:B:236:THR:HG22	2.03	0.40
1:A:931:ILE:O	1:A:934:ILE:HG22	2.20	0.40
1:B:428:ASP:OD1	1:B:428:ASP:N	2.53	0.40
1:C:148:ASN:ND2	10:C:1304:NAG:H81	2.33	0.40
1:A:742:ILE:HG21	1:A:753:LEU:HD12	2.03	0.40
6:R:2:NAG:HO3	6:R:3:BMA:C1	2.32	0.40
1:B:318:PHE:HD1	1:B:595:VAL:HG23	1.86	0.40
1:B:409:GLN:OE1	1:B:417:LYS:N	2.54	0.40
1:C:989:ALA:O	1:C:993:ILE:HG12	2.22	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	1096/1273 (86%)	1032 (94%)	62 (6%)	2 (0%)	47 73
1	B	1096/1273 (86%)	1046 (95%)	44 (4%)	6 (0%)	29 54
1	C	1096/1273 (86%)	1033 (94%)	62 (6%)	1 (0%)	51 78
2	D	124/127 (98%)	120 (97%)	4 (3%)	0	100 100
All	All	3412/3946 (86%)	3231 (95%)	172 (5%)	9 (0%)	44 66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ILE
1	B	534	VAL
1	C	293	LEU
1	B	291	CYS
1	B	591	SER
1	B	592	PHE
1	A	294	ASP
1	B	235	ILE
1	B	632	THR

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	957/1112 (86%)	955 (100%)	2 (0%)	93 98
1	B	958/1112 (86%)	955 (100%)	3 (0%)	92 98
1	C	957/1112 (86%)	954 (100%)	3 (0%)	92 98
2	D	104/105 (99%)	104 (100%)	0	100 100
All	All	2976/3441 (86%)	2968 (100%)	8 (0%)	92 98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	603	ASN

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Mol	Chain	Res	Type
1	B	165	ASN
1	B	278	LYS
1	B	331	ASN
1	C	17	ASN
1	C	234	ASN
1	C	603	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	239	GLN
1	B	804	GLN
1	C	148	ASN
1	C	501	ASN
1	C	804	GLN
1	C	935	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)

81 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.18	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	F	1	4,1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	F	2	4	14,14,15	0.22	0	17,19,21	0.44	0
4	BMA	F	3	4	11,11,12	0.78	0	15,15,17	0.78	0
4	MAN	F	4	4	11,11,12	0.72	1 (9%)	15,15,17	1.09	2 (13%)
4	MAN	F	5	4	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
4	NAG	G	1	4,1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	G	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	BMA	G	3	4	11,11,12	0.56	0	15,15,17	0.75	0
4	MAN	G	4	4	11,11,12	0.64	0	15,15,17	1.10	2 (13%)
4	MAN	G	5	4	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
4	NAG	H	1	4,1	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	H	2	4	14,14,15	0.39	0	17,19,21	0.47	0
4	BMA	H	3	4	11,11,12	0.56	0	15,15,17	0.73	0
4	MAN	H	4	4	11,11,12	1.14	1 (9%)	15,15,17	1.63	3 (20%)
4	MAN	H	5	4	11,11,12	0.64	0	15,15,17	1.15	2 (13%)
5	NAG	I	1	5,1	14,14,15	0.31	0	17,19,21	0.44	0
5	FUC	I	2	5	10,10,11	0.92	0	14,14,16	1.20	1 (7%)
5	GAL	I	3	5	11,11,12	0.81	0	15,15,17	0.98	0
5	FUC	I	4	5	10,10,11	0.65	0	14,14,16	0.81	0
5	NAG	I	5	5	14,14,15	0.28	0	17,19,21	0.47	0
5	BMA	I	6	5	11,11,12	1.00	1 (9%)	15,15,17	0.96	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	J	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	BMA	J	3	4	11,11,12	0.66	0	15,15,17	0.86	0
4	MAN	J	4	4	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
4	MAN	J	5	4	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
3	NAG	K	1	3,1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.53	0
6	NAG	L	1	6,1	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	L	2	6	14,14,15	0.22	0	17,19,21	0.40	0
6	BMA	L	3	6	11,11,12	0.56	0	15,15,17	0.74	0
4	NAG	M	1	4,1	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	M	2	4	14,14,15	0.20	0	17,19,21	0.40	0
4	BMA	M	3	4	11,11,12	0.84	0	15,15,17	0.84	0
4	MAN	M	4	4	11,11,12	1.59	2 (18%)	15,15,17	2.26	4 (26%)
4	MAN	M	5	4	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
7	NAG	N	1	7,1	14,14,15	0.24	0	17,19,21	0.52	0
7	NAG	N	2	7	14,14,15	0.38	0	17,19,21	0.58	0
7	BMA	N	3	7	11,11,12	0.56	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	FUC	N	4	7	10,10,11	0.65	0	14,14,16	0.83	0
4	NAG	O	1	4,1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	O	2	4	14,14,15	0.21	0	17,19,21	0.41	0
4	BMA	O	3	4	11,11,12	0.53	0	15,15,17	0.75	0
4	MAN	O	4	4	11,11,12	0.64	0	15,15,17	1.09	2 (13%)
4	MAN	O	5	4	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
6	NAG	P	1	6,1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	P	2	6	14,14,15	0.21	0	17,19,21	0.40	0
6	BMA	P	3	6	11,11,12	0.56	0	15,15,17	0.75	0
6	NAG	Q	1	6,1	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	Q	2	6	14,14,15	0.21	0	17,19,21	0.41	0
6	BMA	Q	3	6	11,11,12	0.56	0	15,15,17	0.73	0
6	NAG	R	1	6,1	14,14,15	0.40	0	17,19,21	0.72	1 (5%)
6	NAG	R	2	6	14,14,15	0.24	0	17,19,21	0.38	0
6	BMA	R	3	6	11,11,12	0.56	0	15,15,17	0.75	0
3	NAG	S	1	3,1	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	S	2	3	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
3	NAG	T	1	3,1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	T	2	3	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	U	1	6,1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	U	2	6	14,14,15	0.21	0	17,19,21	0.40	0
6	BMA	U	3	6	11,11,12	0.57	0	15,15,17	0.75	0
4	NAG	V	1	4,1	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	V	2	4	14,14,15	0.23	0	17,19,21	0.41	0
4	BMA	V	3	4	11,11,12	0.55	0	15,15,17	0.74	0
4	MAN	V	4	4	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
4	MAN	V	5	4	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
8	NAG	W	1	1,8	14,14,15	0.22	0	17,19,21	0.46	0
8	NAG	W	2	8	14,14,15	0.22	0	17,19,21	0.43	0
8	BMA	W	3	8	11,11,12	1.21	2 (18%)	15,15,17	1.33	2 (13%)
8	MAN	W	4	8	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
9	NAG	X	1	9,1	14,14,15	0.22	0	17,19,21	0.52	0
9	FUC	X	2	9	10,10,11	0.66	0	14,14,16	0.82	0
9	NAG	X	3	9	14,14,15	0.36	0	17,19,21	0.48	0
6	NAG	Y	1	6,1	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	Y	2	6	14,14,15	0.21	0	17,19,21	0.40	0
6	BMA	Y	3	6	11,11,12	0.56	0	15,15,17	0.75	0
6	NAG	Z	1	6,1	14,14,15	0.19	0	17,19,21	0.39	0
6	NAG	Z	2	6	14,14,15	0.22	0	17,19,21	0.47	0
6	BMA	Z	3	6	11,11,12	1.00	1 (9%)	15,15,17	0.94	1 (6%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	MAN	M	4	4	-	1/2/19/22	0/1/1/1
4	MAN	M	5	4	-	0/2/19/22	0/1/1/1
7	NAG	N	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	5/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	FUC	N	4	7	-	-	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
4	MAN	O	4	4	-	0/2/19/22	1/1/1/1
4	MAN	O	5	4	-	1/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	R	2	6	-	1/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
3	NAG	S	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	BMA	V	3	4	-	2/2/19/22	0/1/1/1
4	MAN	V	4	4	-	0/2/19/22	1/1/1/1
4	MAN	V	5	4	-	0/2/19/22	0/1/1/1
8	NAG	W	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
8	BMA	W	3	8	-	1/2/19/22	0/1/1/1
8	MAN	W	4	8	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUC	X	2	9	-	-	0/1/1/1
9	NAG	X	3	9	-	3/6/23/26	0/1/1/1
6	NAG	Y	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	0/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	4	MAN	C1-C2	4.10	1.61	1.52
4	H	4	MAN	C1-C2	3.26	1.59	1.52
4	M	4	MAN	O5-C1	2.95	1.48	1.43
6	Z	3	BMA	C1-C2	2.70	1.58	1.52
5	I	6	BMA	C1-C2	2.66	1.58	1.52
8	W	3	BMA	C2-C3	2.64	1.56	1.52
8	W	3	BMA	C1-C2	2.15	1.57	1.52
4	F	4	MAN	C1-C2	2.01	1.56	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	4	MAN	C1-O5-C5	6.34	120.78	112.19
4	H	4	MAN	C1-O5-C5	4.38	118.13	112.19
4	M	4	MAN	C1-C2-C3	3.55	114.03	109.67
4	M	4	MAN	O5-C1-C2	3.45	116.10	110.77
3	S	2	NAG	C1-O5-C5	3.36	116.75	112.19
8	W	3	BMA	C1-C2-C3	3.17	113.56	109.67
5	I	2	FUC	O5-C5-C4	2.96	114.82	109.52
4	V	4	MAN	C1-O5-C5	2.90	116.12	112.19
4	F	4	MAN	C1-O5-C5	2.90	116.12	112.19
4	G	4	MAN	C1-O5-C5	2.89	116.11	112.19
4	O	4	MAN	C1-O5-C5	2.84	116.04	112.19
4	J	4	MAN	C1-O5-C5	2.74	115.91	112.19
4	H	5	MAN	C1-O5-C5	2.67	115.80	112.19
4	H	4	MAN	C1-C2-C3	2.64	112.91	109.67
8	W	3	BMA	C2-C3-C4	2.43	115.09	110.89
5	I	6	BMA	O2-C2-C3	-2.41	105.31	110.14
8	W	4	MAN	C1-O5-C5	2.36	115.39	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	3	BMA	O2-C2-C3	-2.33	105.47	110.14
4	M	4	MAN	O2-C2-C3	-2.27	105.59	110.14
4	H	4	MAN	O2-C2-C3	-2.24	105.65	110.14
4	O	5	MAN	C1-O5-C5	2.24	115.23	112.19
4	J	5	MAN	C1-O5-C5	2.23	115.22	112.19
8	W	4	MAN	O2-C2-C3	-2.22	105.69	110.14
4	O	4	MAN	O2-C2-C3	-2.22	105.69	110.14
4	V	5	MAN	O2-C2-C3	-2.22	105.69	110.14
4	J	5	MAN	O2-C2-C3	-2.22	105.70	110.14
4	O	5	MAN	O2-C2-C3	-2.21	105.70	110.14
4	G	5	MAN	O2-C2-C3	-2.21	105.70	110.14
4	M	5	MAN	O2-C2-C3	-2.21	105.70	110.14
4	F	5	MAN	O2-C2-C3	-2.21	105.70	110.14
4	H	5	MAN	O2-C2-C3	-2.21	105.71	110.14
4	V	4	MAN	O2-C2-C3	-2.20	105.72	110.14
4	G	4	MAN	O2-C2-C3	-2.20	105.73	110.14
4	M	5	MAN	C1-O5-C5	2.19	115.17	112.19
4	V	5	MAN	C1-O5-C5	2.19	115.17	112.19
4	J	4	MAN	O2-C2-C3	-2.19	105.74	110.14
4	F	5	MAN	C1-O5-C5	2.18	115.15	112.19
4	G	5	MAN	C1-O5-C5	2.18	115.15	112.19
4	F	4	MAN	O2-C2-C3	-2.17	105.78	110.14
6	R	1	NAG	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	O	3	BMA	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
8	W	1	NAG	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
9	X	1	NAG	C8-C7-N2-C2
9	X	1	NAG	O7-C7-N2-C2
6	L	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
8	W	2	NAG	O5-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
8	W	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
9	X	3	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	S	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
8	W	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	M	4	MAN	O5-C5-C6-O6
5	I	6	BMA	O5-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	O	5	MAN	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
9	X	3	NAG	O5-C5-C6-O6
4	V	3	BMA	O5-C5-C6-O6
4	V	3	BMA	C4-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7
3	S	1	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7
4	H	2	NAG	C3-C2-N2-C7
4	M	2	NAG	C3-C2-N2-C7
5	I	5	NAG	C3-C2-N2-C7
6	L	2	NAG	C3-C2-N2-C7
6	P	2	NAG	C3-C2-N2-C7
6	Q	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7
6	R	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	Z	2	NAG	C3-C2-N2-C7
7	N	2	NAG	C3-C2-N2-C7
9	X	3	NAG	C3-C2-N2-C7
4	J	5	MAN	O5-C5-C6-O6
4	J	5	MAN	C4-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
4	O	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7
9	X	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C1-C2-N2-C7

All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	5	MAN	C1-C2-C3-C4-C5-O5
4	J	4	MAN	C1-C2-C3-C4-C5-O5
4	V	4	MAN	C1-C2-C3-C4-C5-O5
4	G	4	MAN	C1-C2-C3-C4-C5-O5
4	O	4	MAN	C1-C2-C3-C4-C5-O5
4	F	4	MAN	C1-C2-C3-C4-C5-O5

56 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	2	NAG	7	0
6	Z	2	NAG	4	0
4	F	1	NAG	5	0
5	I	6	BMA	4	0
8	W	3	BMA	2	0
4	M	5	MAN	1	0
4	M	1	NAG	4	0
3	T	2	NAG	1	0
6	L	2	NAG	1	0
4	M	3	BMA	6	0
4	V	3	BMA	3	0
6	R	3	BMA	2	0
6	P	2	NAG	1	0
4	G	3	BMA	1	0
4	F	3	BMA	4	0
8	W	4	MAN	1	0
3	S	2	NAG	4	0

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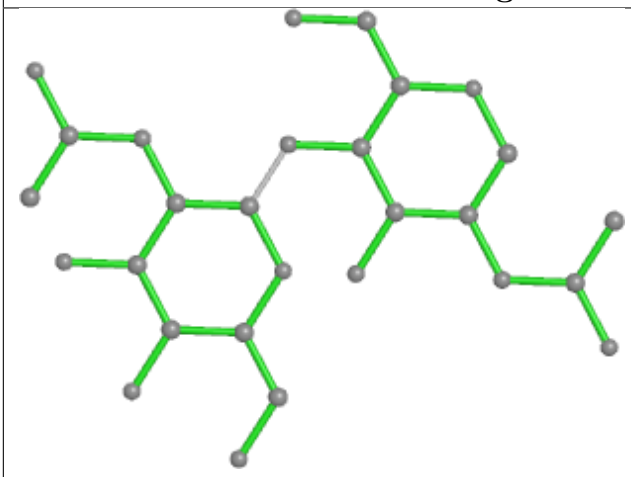
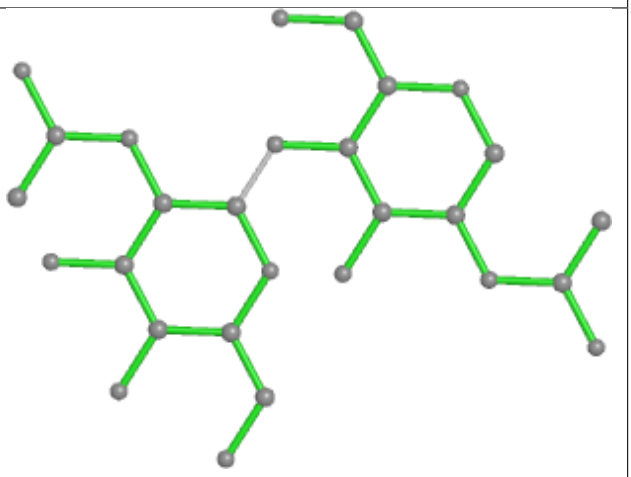
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Y	1	NAG	3	0
4	G	5	MAN	1	0
6	Z	3	BMA	4	0
8	W	2	NAG	2	0
4	F	5	MAN	1	0
4	O	1	NAG	2	0
9	X	3	NAG	6	0
4	J	5	MAN	1	0
9	X	2	FUC	2	0
6	R	2	NAG	6	0
4	H	2	NAG	3	0
4	O	3	BMA	4	0
3	E	1	NAG	2	0
9	X	1	NAG	4	0
4	H	3	BMA	5	0
4	O	5	MAN	2	0
4	V	2	NAG	1	0
6	R	1	NAG	9	0
4	H	1	NAG	8	0
4	O	2	NAG	3	0
4	F	2	NAG	1	0
3	K	2	NAG	4	0
8	W	1	NAG	1	0
7	N	4	FUC	1	0
5	I	5	NAG	4	0
4	H	4	MAN	5	0
6	L	1	NAG	1	0
5	I	2	FUC	1	0
7	N	1	NAG	2	0
3	S	1	NAG	6	0
4	F	4	MAN	3	0
4	G	2	NAG	1	0
4	J	1	NAG	1	0
3	E	2	NAG	1	0
4	M	4	MAN	5	0
3	T	1	NAG	1	0
4	V	5	MAN	2	0
5	I	1	NAG	2	0
4	J	3	BMA	1	0

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

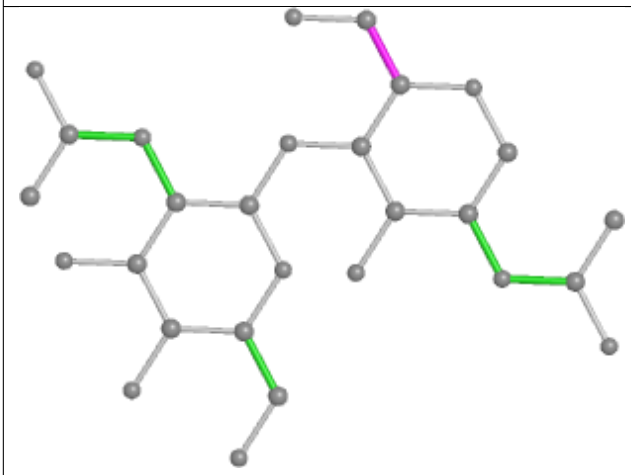
Oligosaccharide Chain E



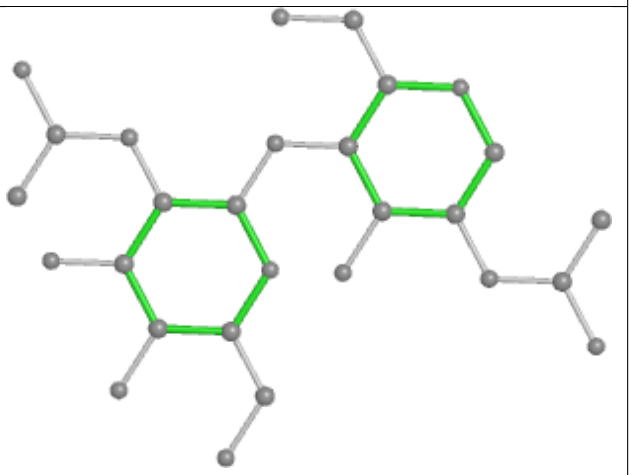
Bond lengths



Bond angles

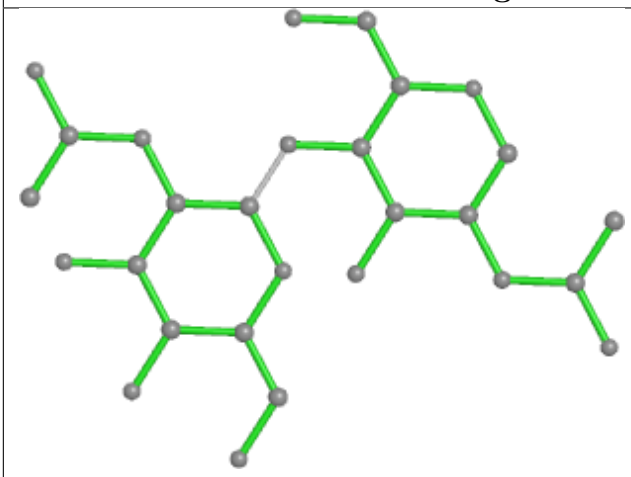


Torsions

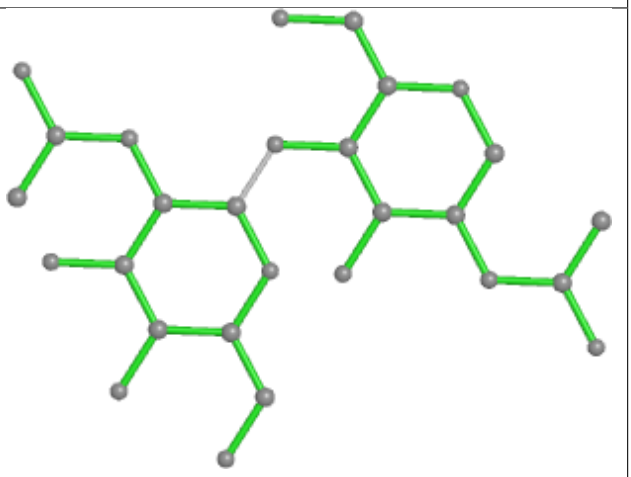


Rings

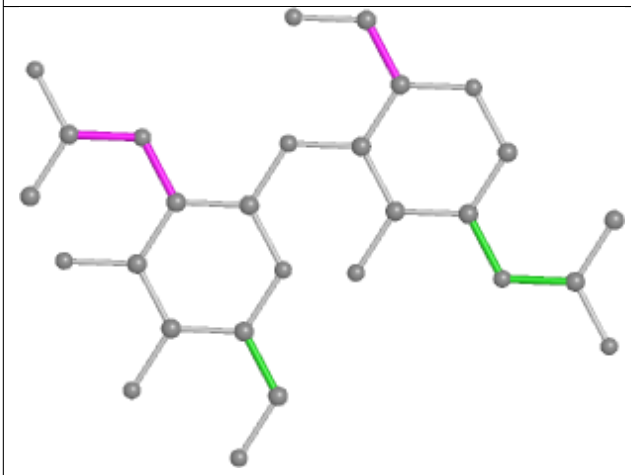
Oligosaccharide Chain K



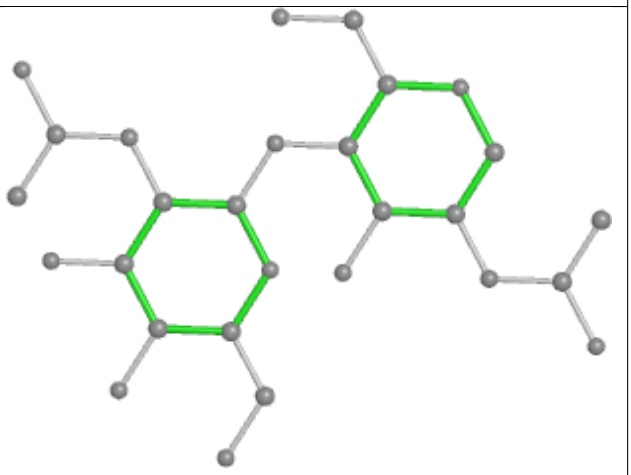
Bond lengths



Bond angles

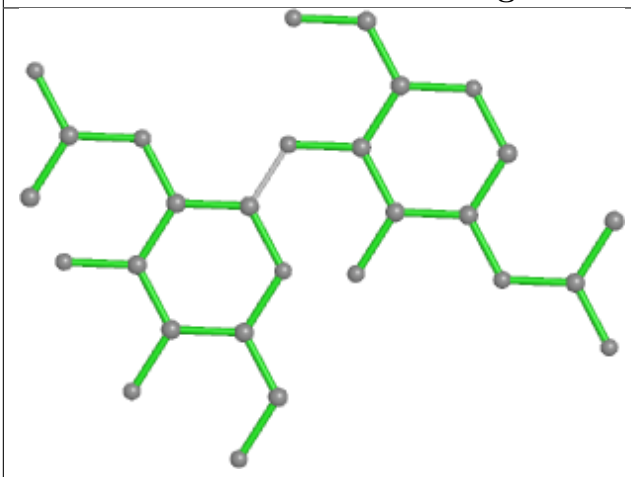


Torsions

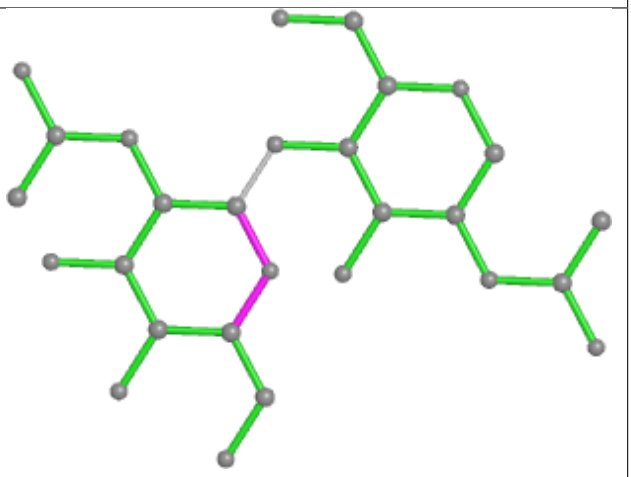


Rings

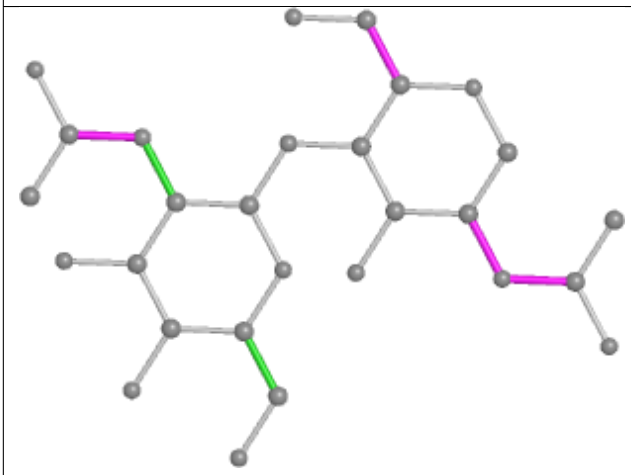
Oligosaccharide Chain S



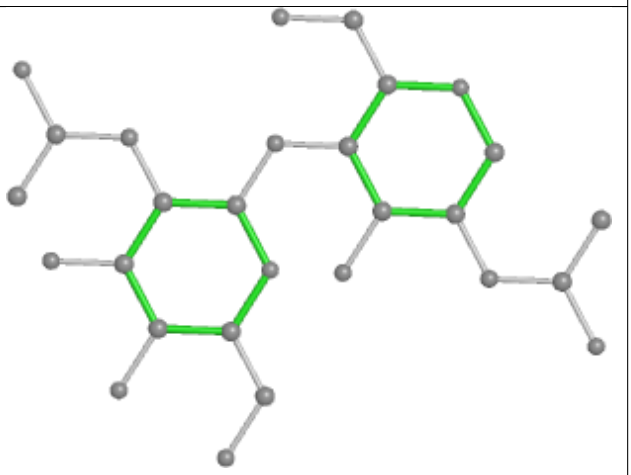
Bond lengths



Bond angles

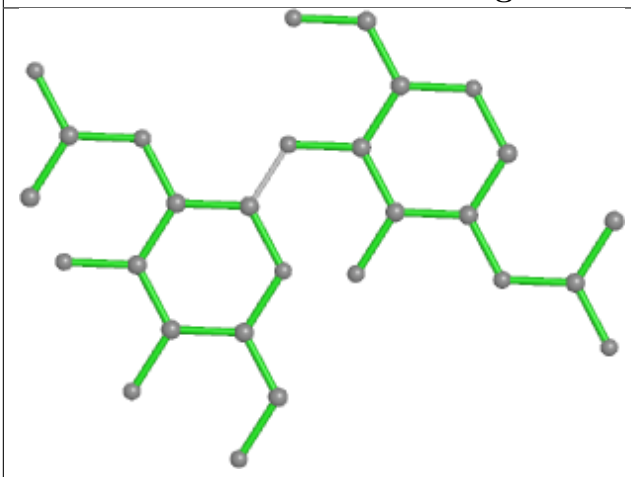


Torsions

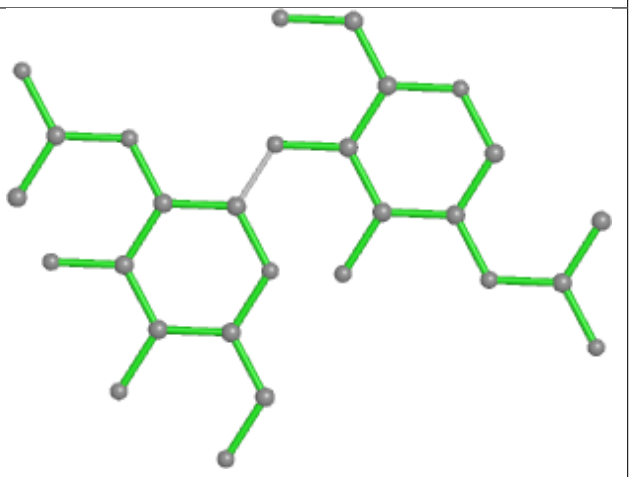


Rings

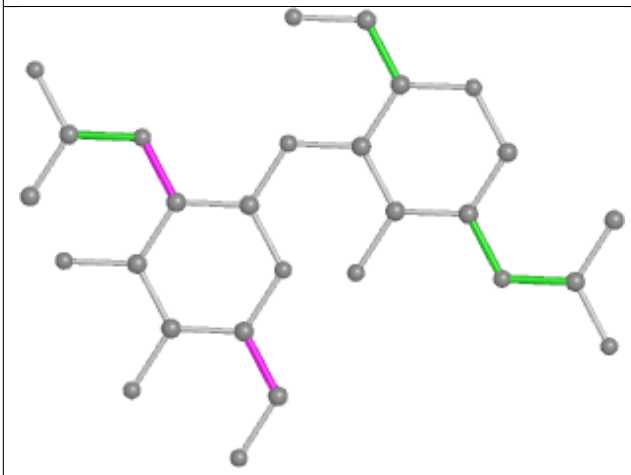
Oligosaccharide Chain T



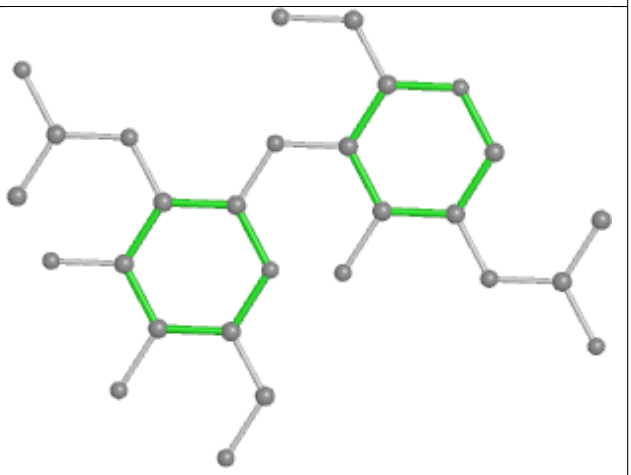
Bond lengths



Bond angles

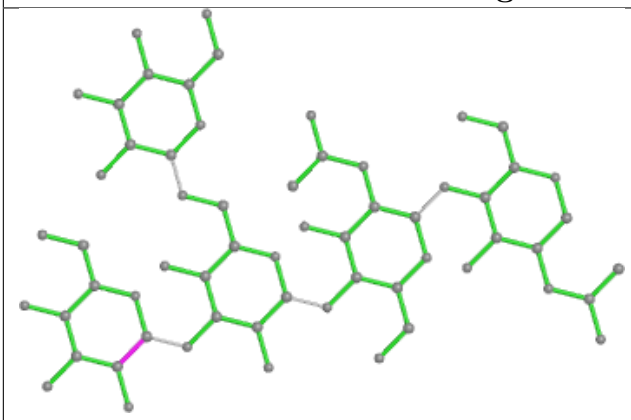


Torsions

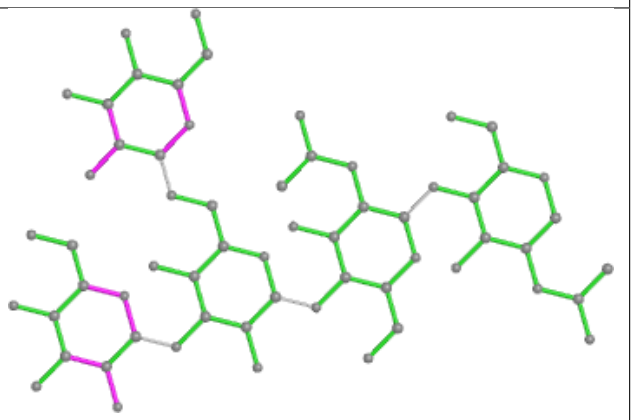


Rings

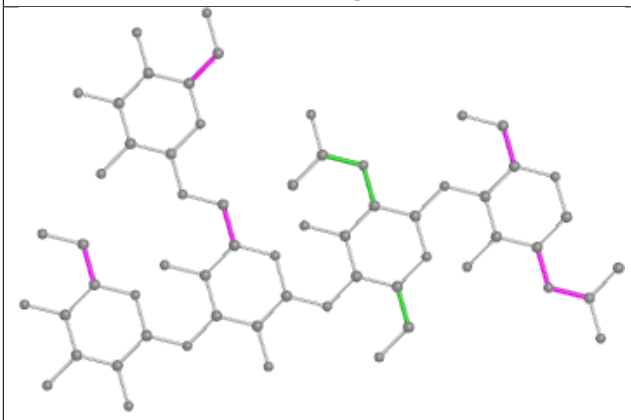
Oligosaccharide Chain F



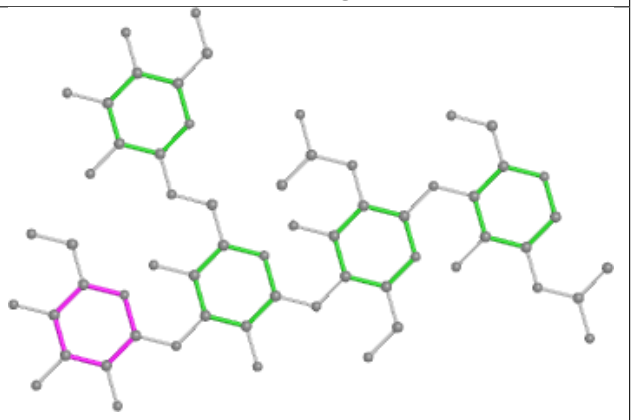
Bond lengths



Bond angles

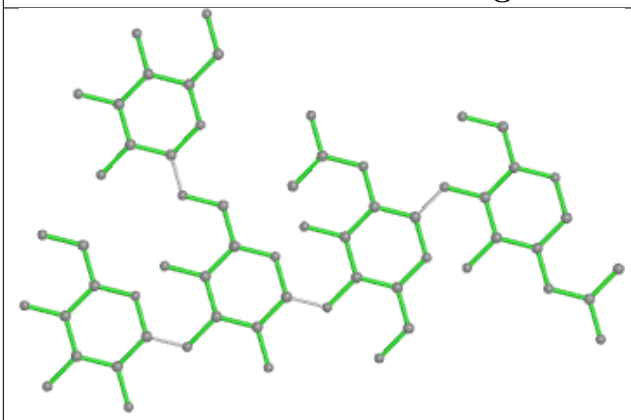


Torsions

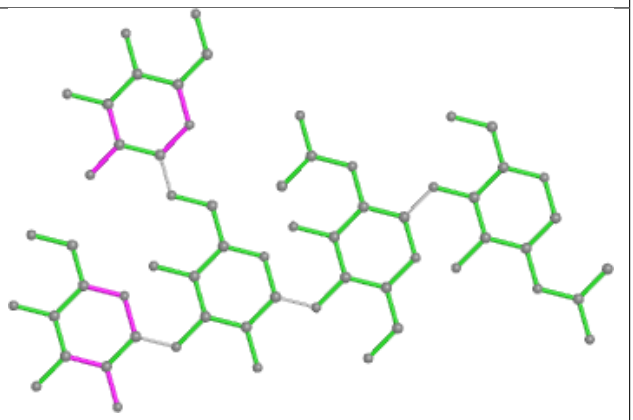


Rings

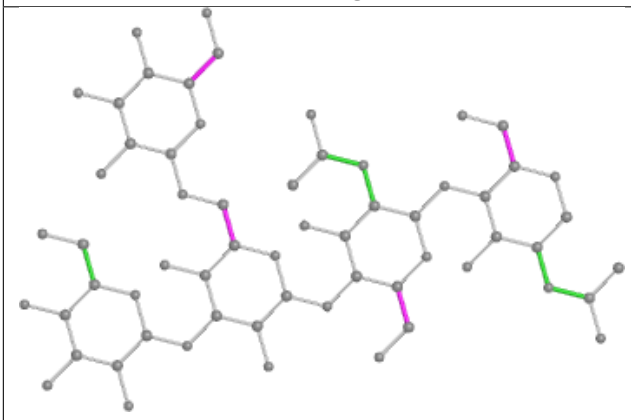
Oligosaccharide Chain G



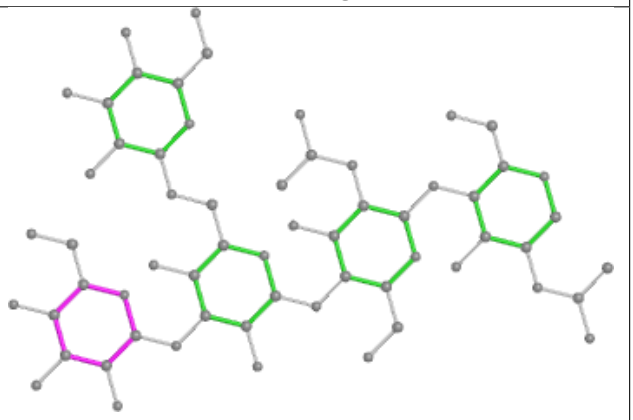
Bond lengths



Bond angles

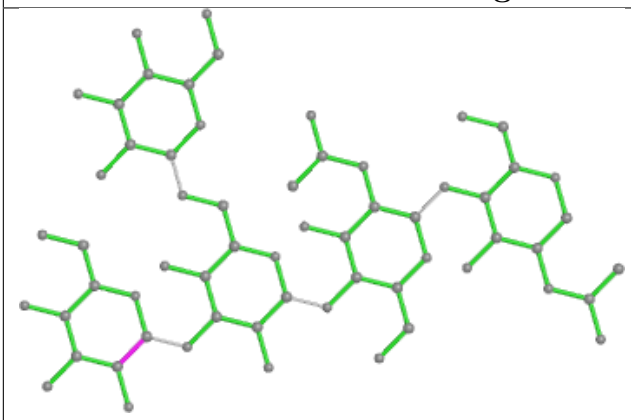


Torsions

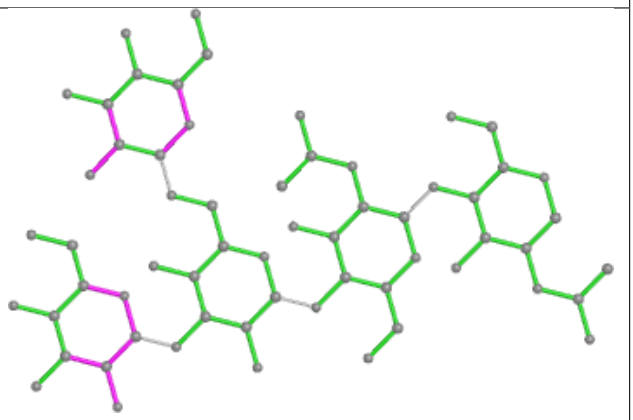


Rings

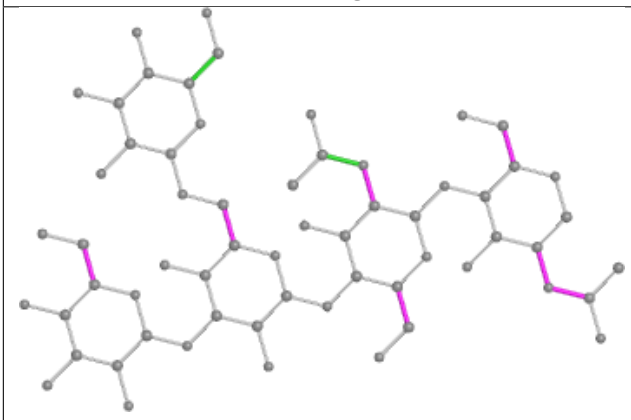
Oligosaccharide Chain H



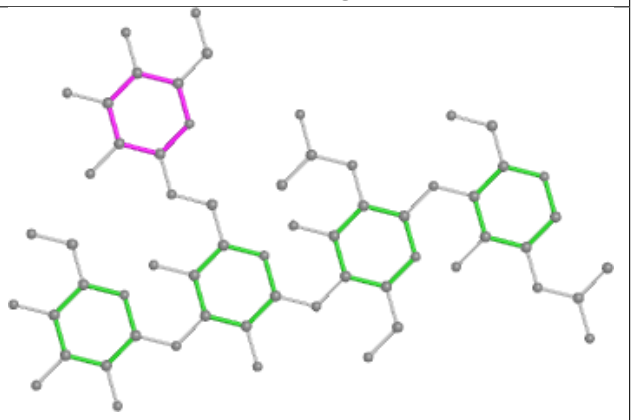
Bond lengths



Bond angles

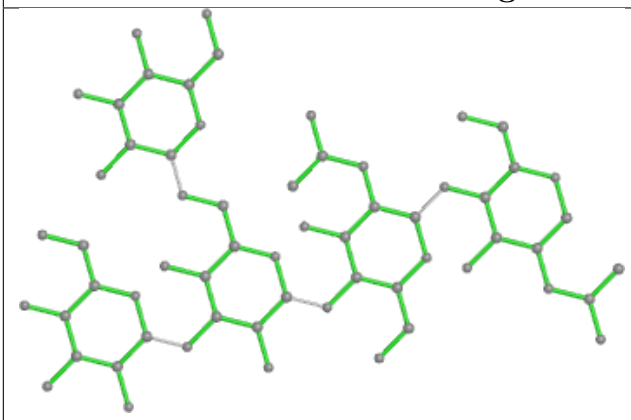


Torsions

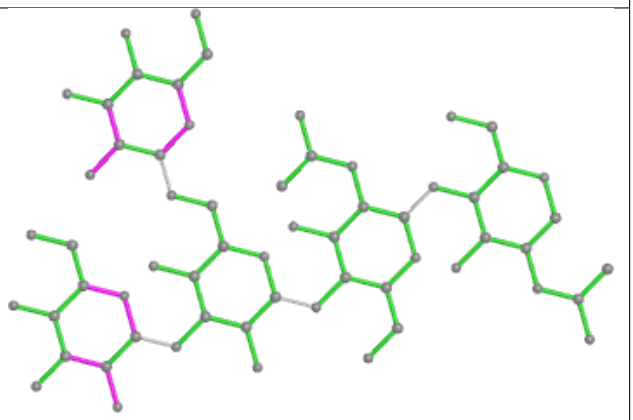


Rings

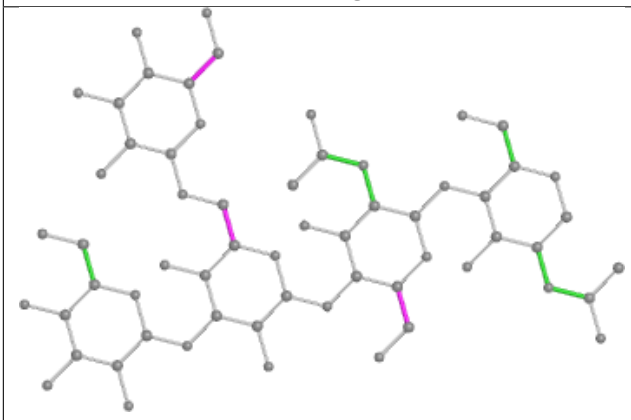
Oligosaccharide Chain J



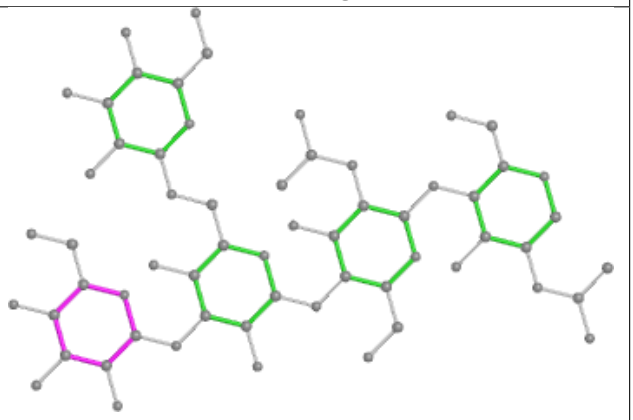
Bond lengths



Bond angles

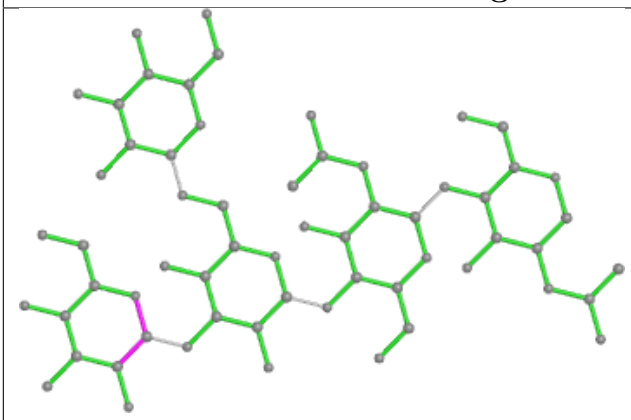


Torsions



Rings

Oligosaccharide Chain M



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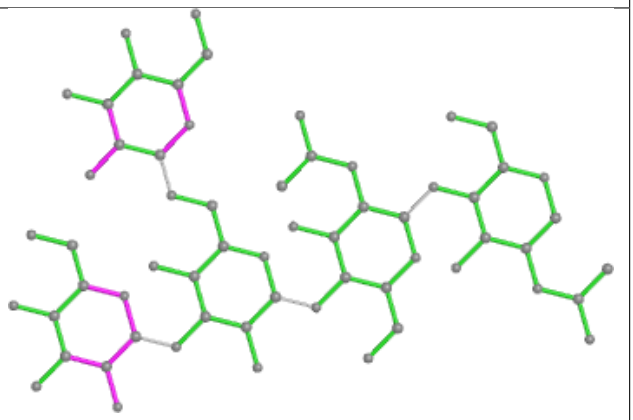
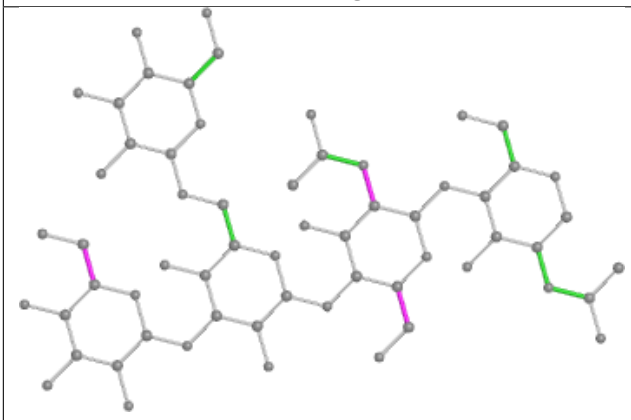


Bond angles



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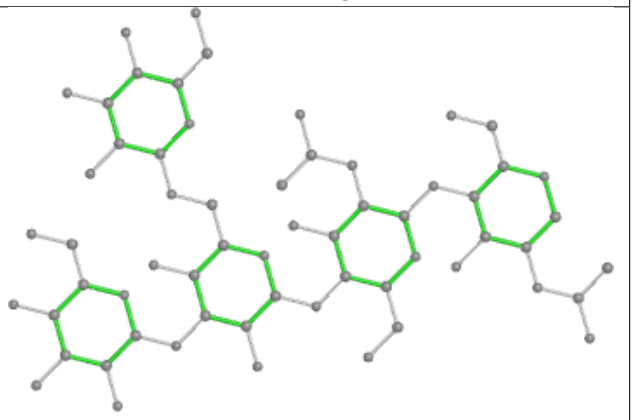
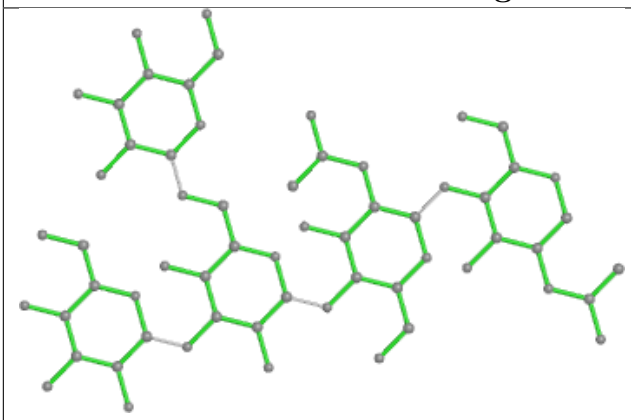


Rings

Oligosaccharide Chain O



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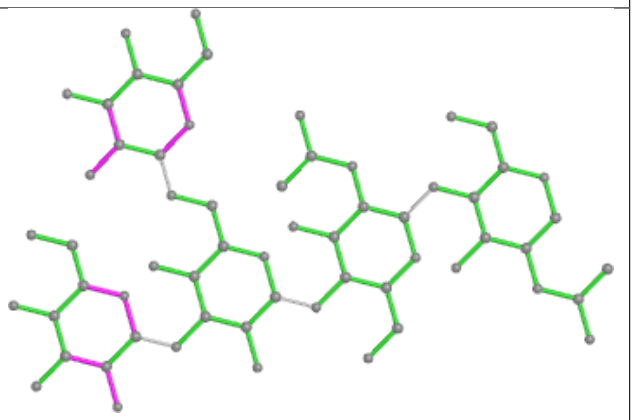
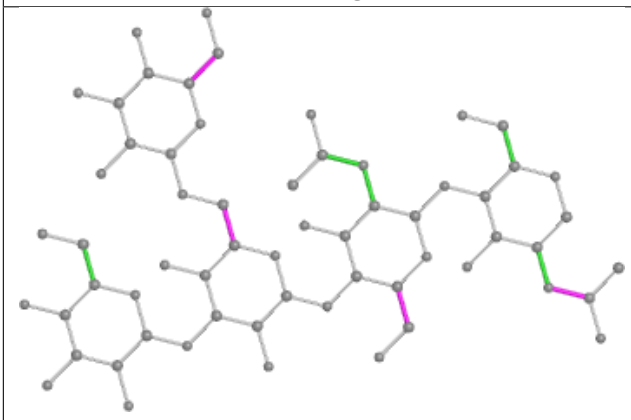
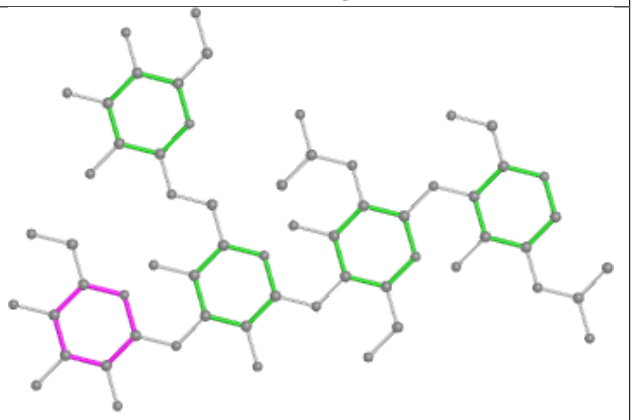


Bond angles

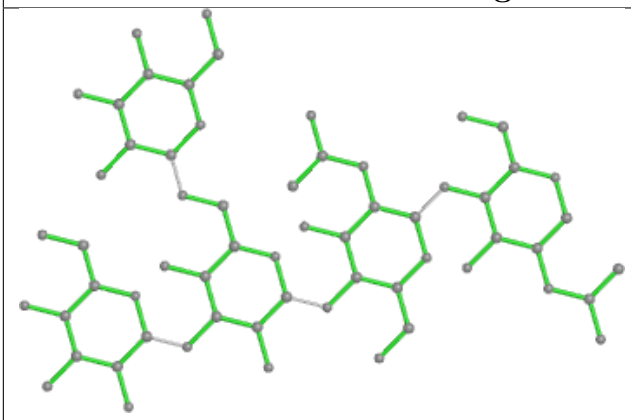


Torsions



Rings

Oligosaccharide Chain V



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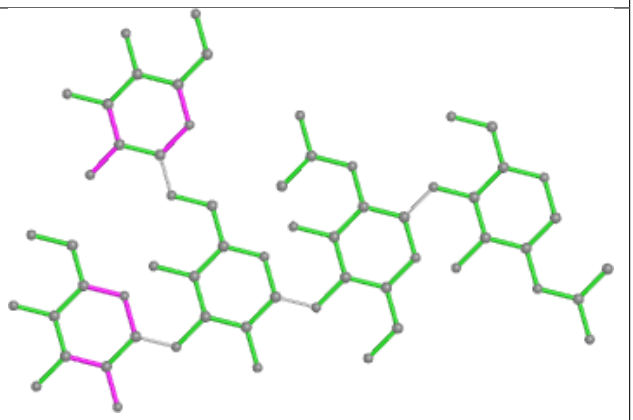
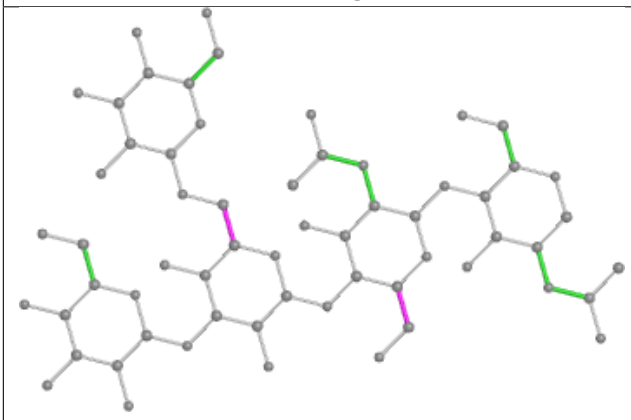
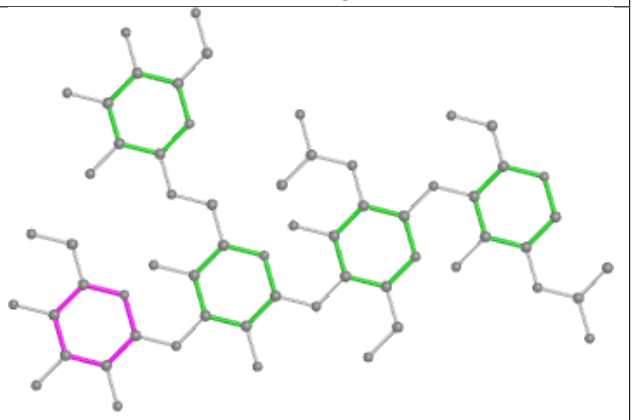


Bond angles

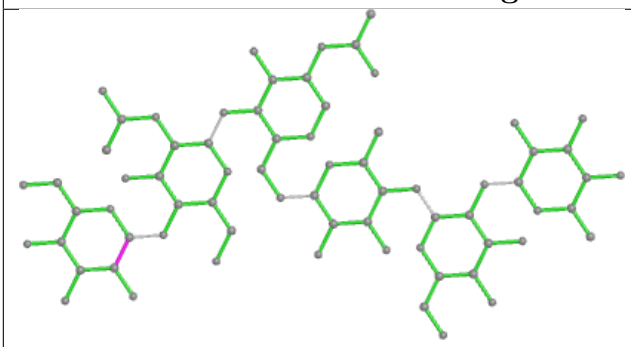


Torsions

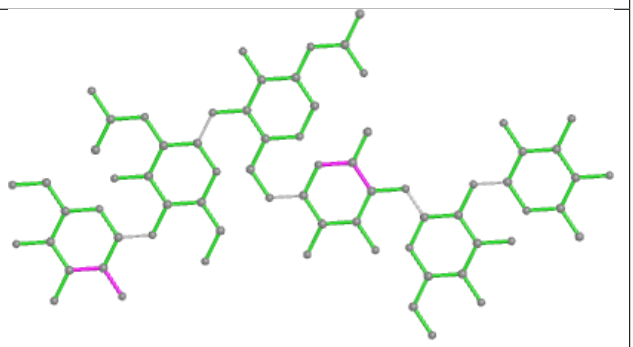


Rings

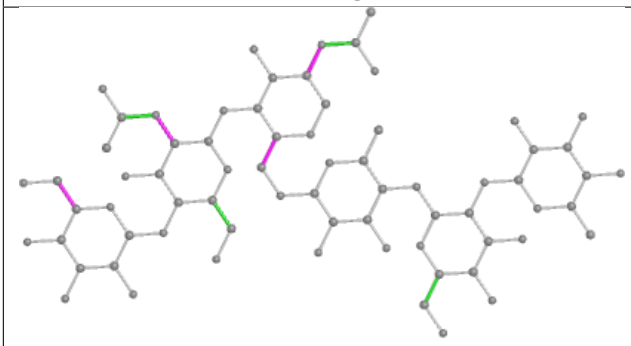
Oligosaccharide Chain I



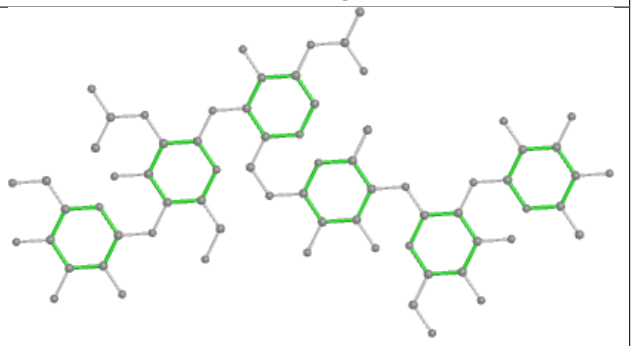
Bond lengths



Bond angles

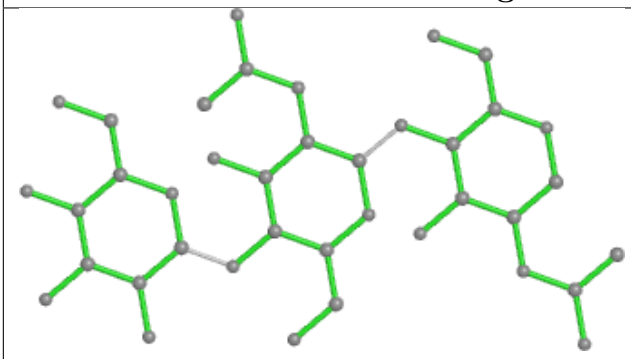


Torsions



Rings

Oligosaccharide Chain L



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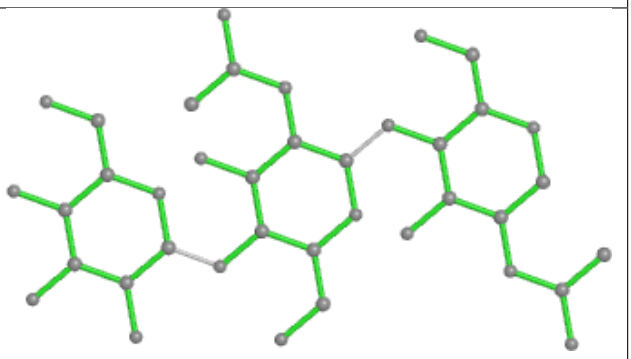
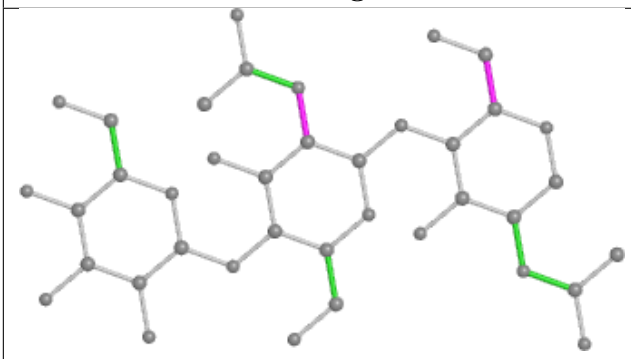


Bond angles



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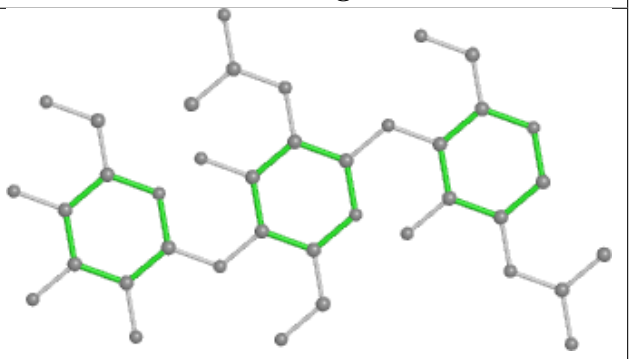
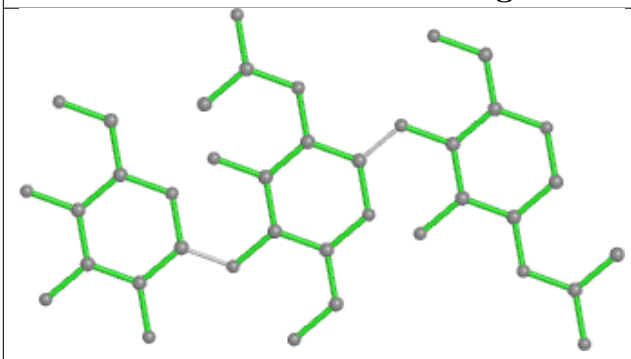


Rings

Oligosaccharide Chain P



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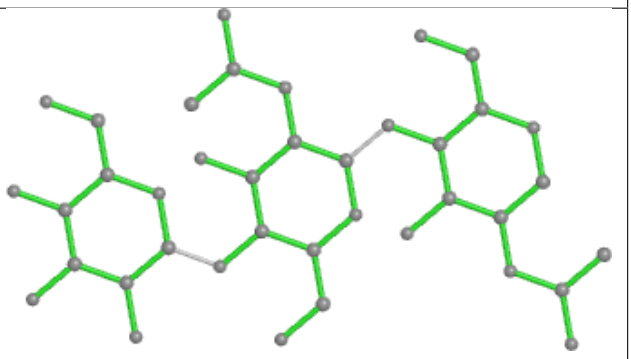
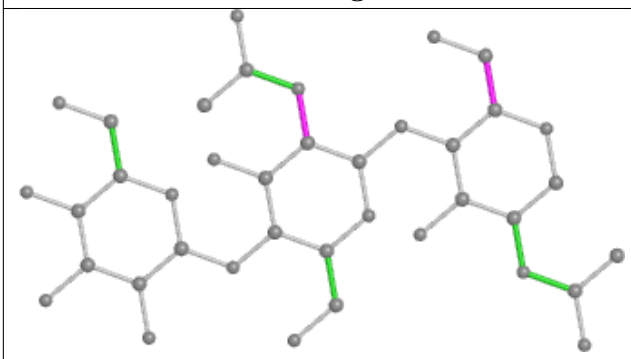


Bond angles



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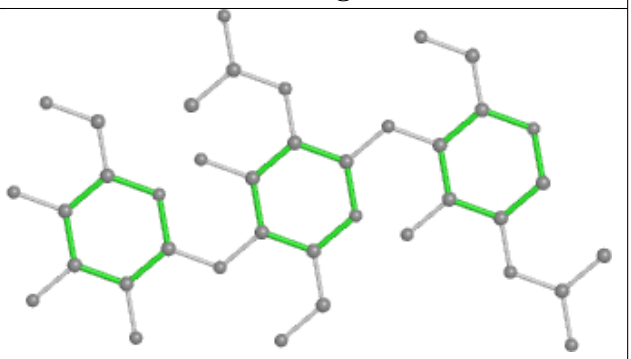
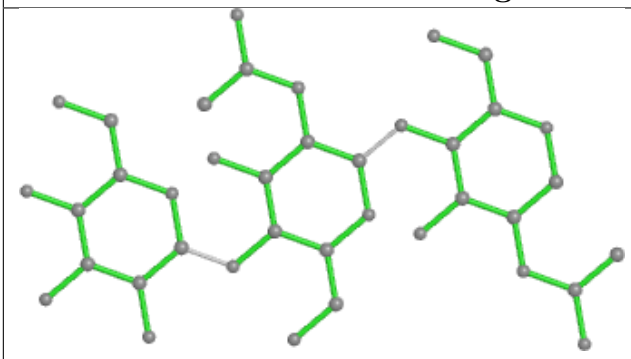


Rings

Oligosaccharide Chain Q



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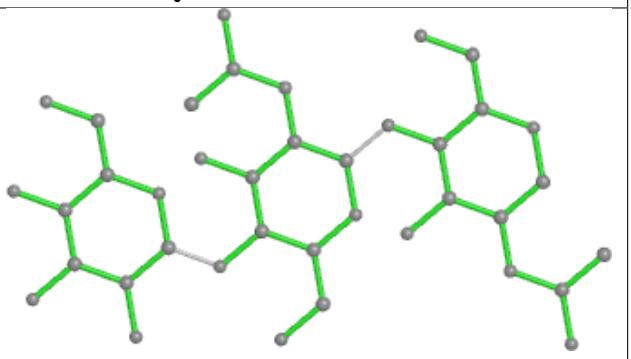
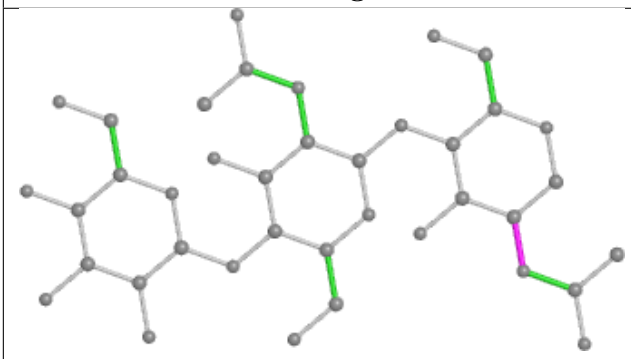
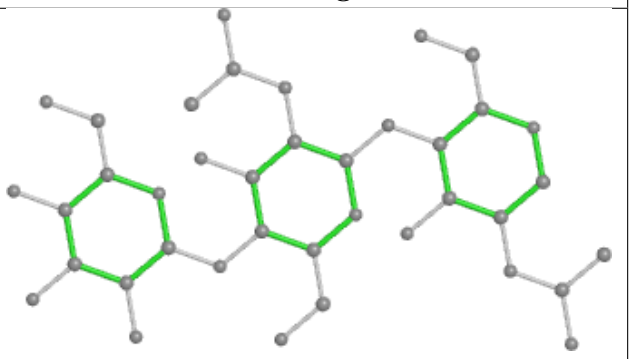


Bond angles

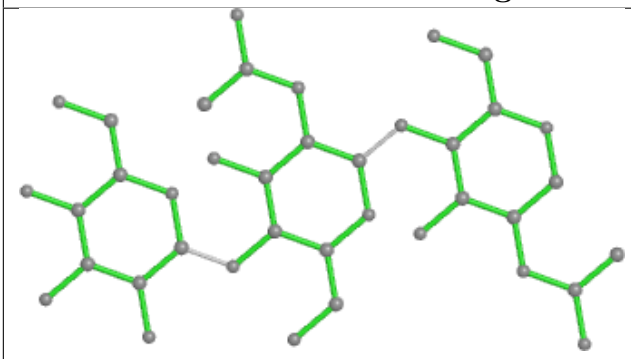


Torsions



Rings

Oligosaccharide Chain R



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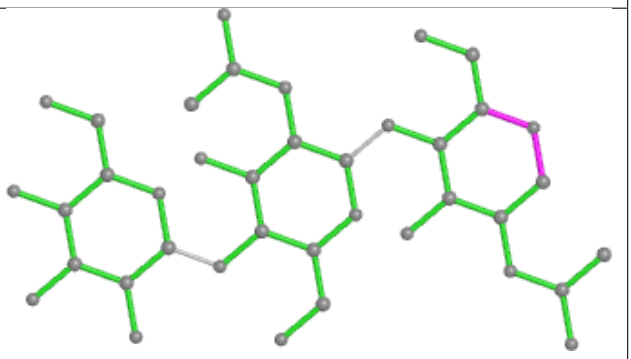
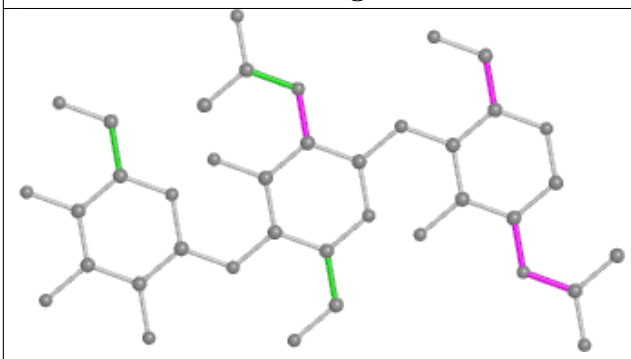
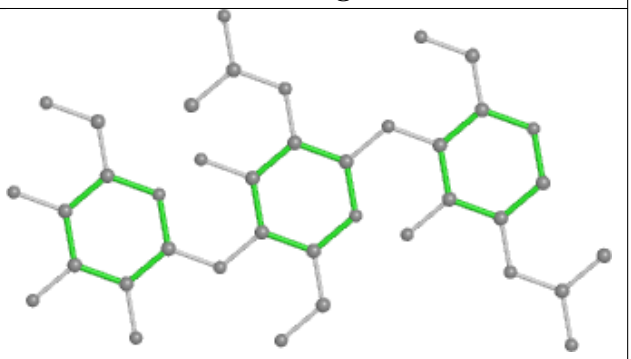


Bond angles

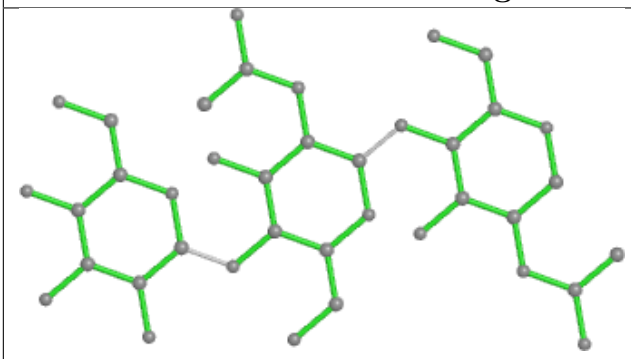


Torsions

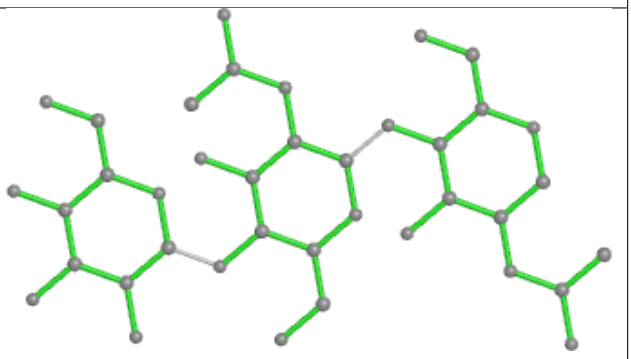


Rings

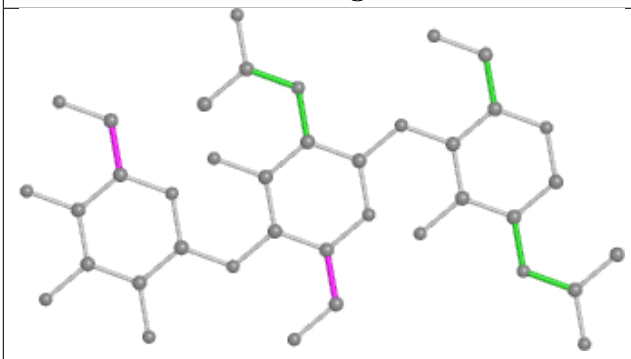
Oligosaccharide Chain U



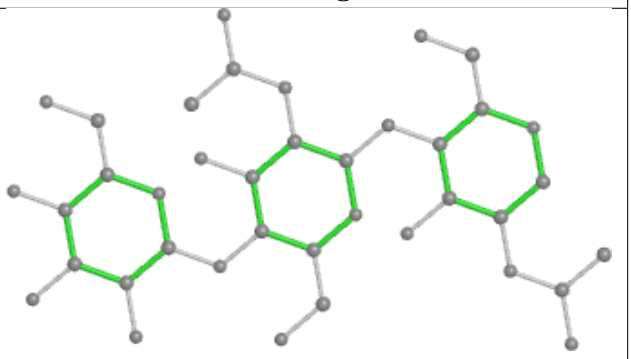
Bond lengths



Bond angles

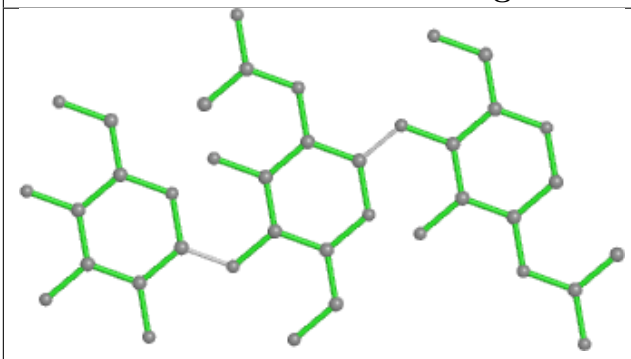


Torsions



Rings

Oligosaccharide Chain Y



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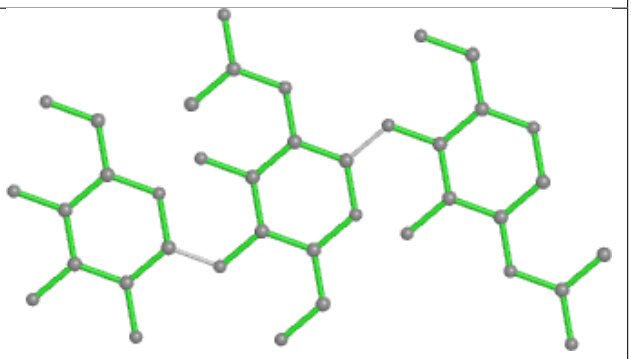
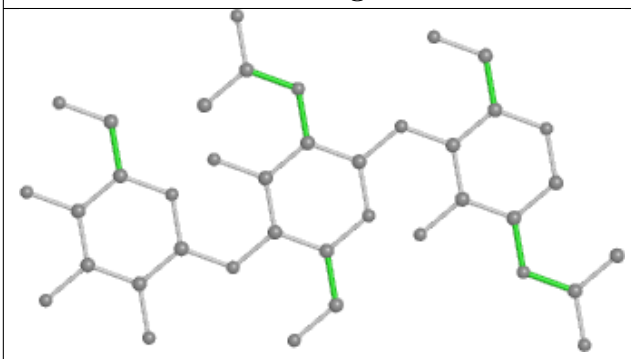
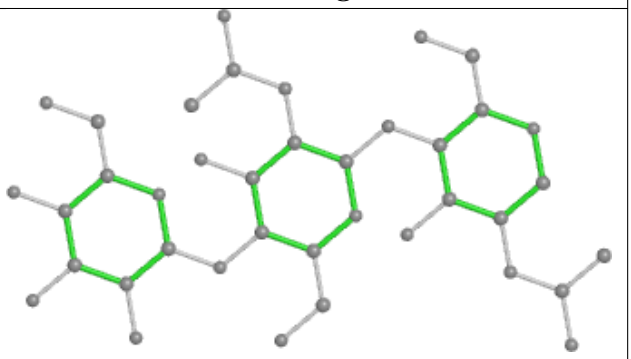


Bond angles

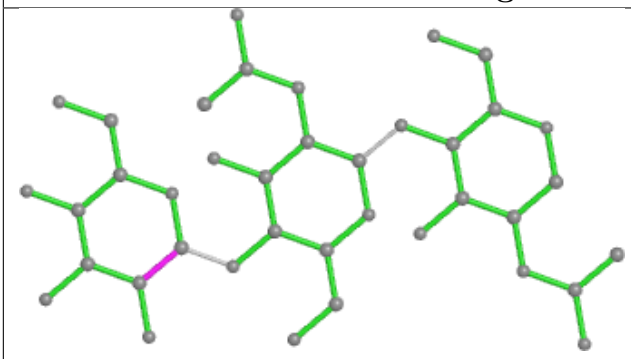


Torsions



Rings

Oligosaccharide Chain Z



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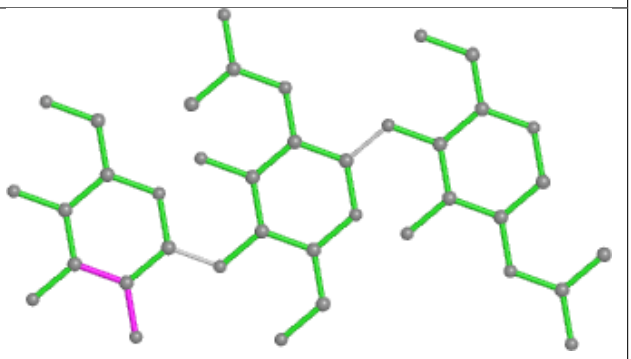
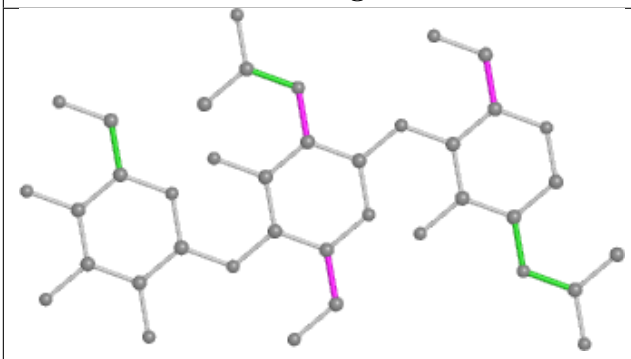


Bond angles



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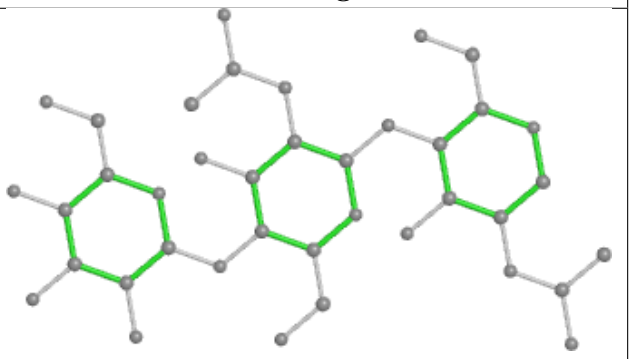
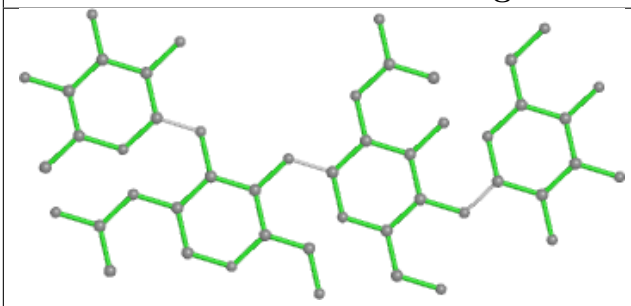
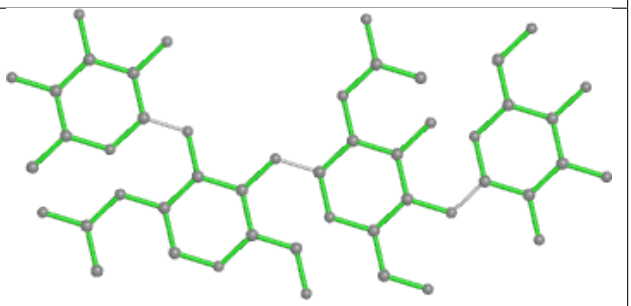


Rings

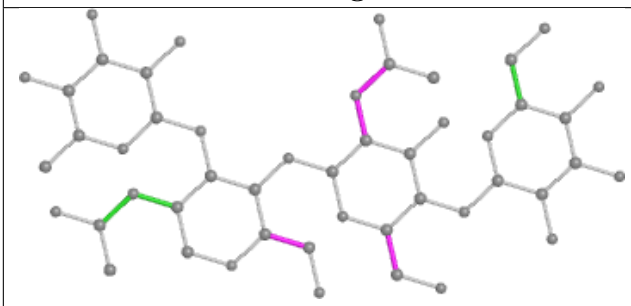
Oligosaccharide Chain N



Bond lengths



Bond angles



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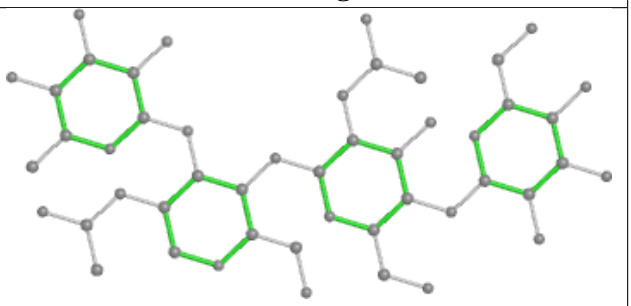
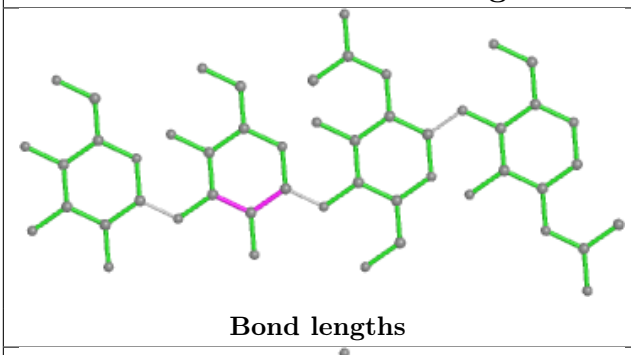
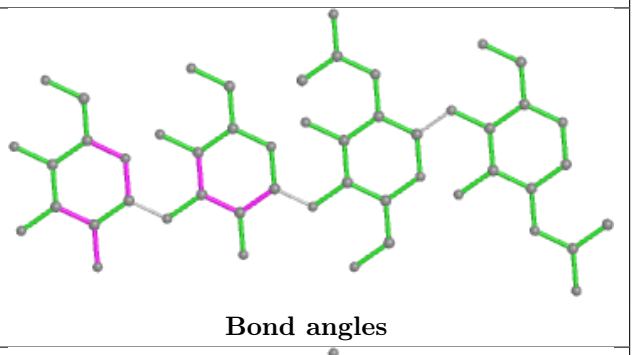


Rings

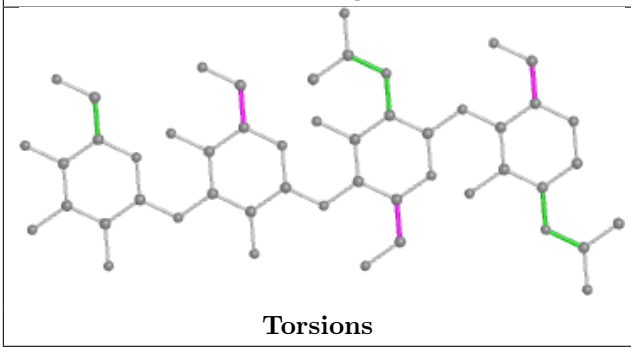
Oligosaccharide Chain W



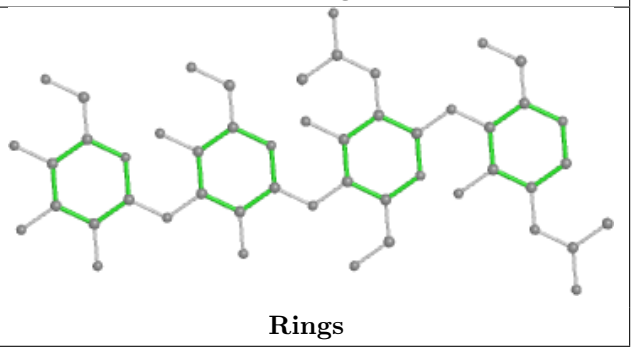
Bond lengths



Bond angles

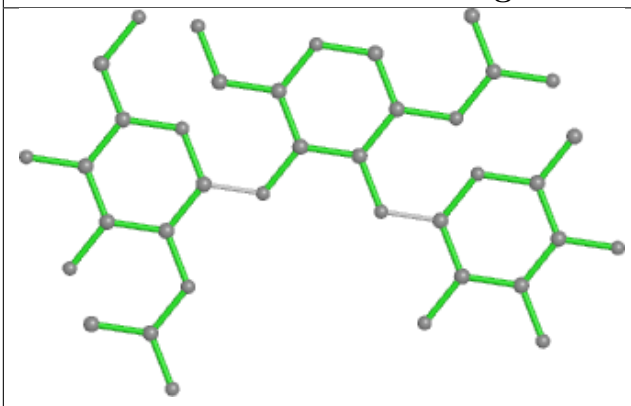


Torsions

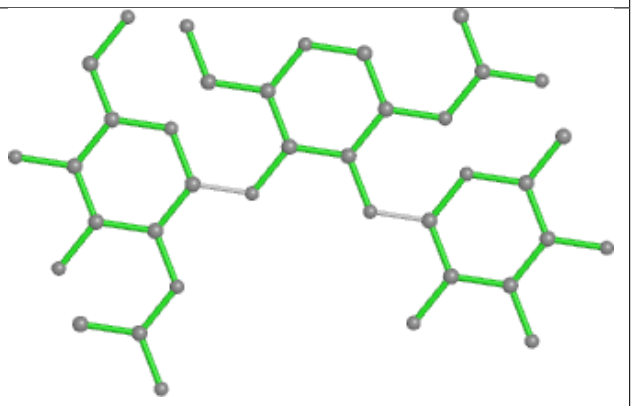


Rings

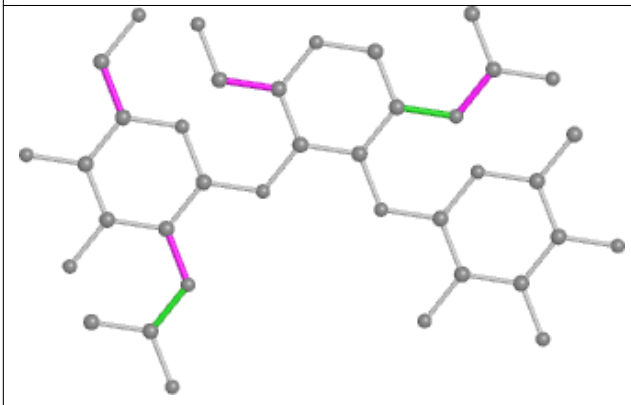
Oligosaccharide Chain X



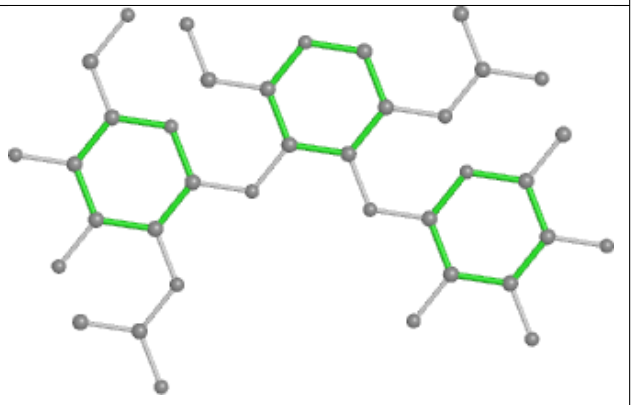
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

33 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	$\#\|Z\| > 2$
10	NAG	C	1309	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	C	1310	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	B	1307	1	14,14,15	0.20	0	17,19,21	0.41	0
10	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.41	0
11	AH2	A	1312	-	11,11,11	0.59	0	15,15,15	0.79	0
10	NAG	C	1306	1	14,14,15	0.23	0	17,19,21	0.39	0
10	NAG	B	1310	1	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	C	1304	1	14,14,15	0.27	0	17,19,21	0.85	1 (5%)
10	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.39	0
10	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	B	1301	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	B	1311	1	14,14,15	0.24	0	17,19,21	0.53	0
10	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.39	0
10	NAG	B	1303	1	14,14,15	0.53	0	17,19,21	0.50	0
10	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.39	0
10	NAG	A	1308	1	14,14,15	0.24	0	17,19,21	0.39	0
10	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	B	1308	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	A	1310	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.42	0
10	NAG	A	1311	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.38	0
10	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.40	0
10	NAG	B	1309	1	14,14,15	0.21	0	17,19,21	0.39	0
10	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.53	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
10	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
10	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
10	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
10	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
11	AH2	A	1312	-	-	0/2/19/19	0/1/1/1
10	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
10	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1304	1	-	5/6/23/26	0/1/1/1
10	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
10	NAG	B	1311	1	-	3/6/23/26	0/1/1/1
10	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
10	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
10	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1308	1	-	4/6/23/26	0/1/1/1
10	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
10	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
10	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
10	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
10	NAG	B	1309	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
10	NAG	B	1305	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1304	NAG	C1-O5-C5	2.76	115.93	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1304	NAG	C4-C5-C6-O6
10	B	1309	NAG	C4-C5-C6-O6
10	B	1306	NAG	O5-C5-C6-O6
10	C	1304	NAG	C4-C5-C6-O6
10	B	1309	NAG	O5-C5-C6-O6
10	C	1306	NAG	O5-C5-C6-O6
10	B	1304	NAG	O5-C5-C6-O6
10	B	1303	NAG	O5-C5-C6-O6
10	B	1305	NAG	O5-C5-C6-O6
10	A	1306	NAG	O5-C5-C6-O6
10	C	1306	NAG	C4-C5-C6-O6
10	C	1308	NAG	O5-C5-C6-O6
10	B	1308	NAG	O5-C5-C6-O6
10	A	1302	NAG	C4-C5-C6-O6
10	A	1308	NAG	C4-C5-C6-O6
10	C	1304	NAG	O5-C5-C6-O6
10	B	1306	NAG	C4-C5-C6-O6
10	A	1308	NAG	C1-C2-N2-C7
10	B	1305	NAG	C4-C5-C6-O6
10	A	1301	NAG	O5-C5-C6-O6
10	B	1308	NAG	C4-C5-C6-O6
10	A	1302	NAG	C8-C7-N2-C2
10	A	1302	NAG	O7-C7-N2-C2
10	A	1306	NAG	C8-C7-N2-C2
10	A	1306	NAG	O7-C7-N2-C2
10	B	1305	NAG	C8-C7-N2-C2
10	B	1305	NAG	O7-C7-N2-C2
10	B	1307	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
10	B	1307	NAG	O7-C7-N2-C2
10	B	1308	NAG	C8-C7-N2-C2
10	B	1308	NAG	O7-C7-N2-C2
10	B	1311	NAG	C8-C7-N2-C2
10	B	1311	NAG	O7-C7-N2-C2
10	C	1303	NAG	C8-C7-N2-C2
10	C	1303	NAG	O7-C7-N2-C2
10	C	1304	NAG	C8-C7-N2-C2
10	C	1304	NAG	O7-C7-N2-C2
10	C	1308	NAG	C4-C5-C6-O6
10	A	1302	NAG	O5-C5-C6-O6
10	A	1308	NAG	O5-C5-C6-O6
10	B	1303	NAG	C4-C5-C6-O6
10	A	1306	NAG	C4-C5-C6-O6
10	A	1310	NAG	O5-C5-C6-O6
10	B	1310	NAG	O5-C5-C6-O6
10	B	1310	NAG	C4-C5-C6-O6
10	A	1307	NAG	O5-C5-C6-O6
10	C	1303	NAG	O5-C5-C6-O6
10	C	1305	NAG	O5-C5-C6-O6
10	A	1301	NAG	C4-C5-C6-O6
10	C	1301	NAG	C4-C5-C6-O6
10	B	1303	NAG	C1-C2-N2-C7
10	B	1301	NAG	C4-C5-C6-O6
10	A	1308	NAG	C3-C2-N2-C7
10	B	1305	NAG	C3-C2-N2-C7
10	B	1311	NAG	C3-C2-N2-C7
10	C	1304	NAG	C3-C2-N2-C7
10	C	1307	NAG	C3-C2-N2-C7
10	C	1309	NAG	C3-C2-N2-C7
10	A	1311	NAG	C4-C5-C6-O6
10	A	1310	NAG	C4-C5-C6-O6
10	C	1301	NAG	O5-C5-C6-O6
10	B	1303	NAG	C3-C2-N2-C7
10	A	1304	NAG	C4-C5-C6-O6
10	C	1307	NAG	C1-C2-N2-C7

There are no ring outliers.

16 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1301	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1307	NAG	2	0
10	C	1301	NAG	2	0
10	A	1304	NAG	1	0
10	C	1306	NAG	1	0
10	C	1304	NAG	6	0
10	A	1303	NAG	1	0
10	A	1305	NAG	1	0
10	B	1311	NAG	4	0
10	A	1302	NAG	1	0
10	B	1303	NAG	1	0
10	B	1306	NAG	1	0
10	A	1308	NAG	2	0
10	B	1308	NAG	2	0
10	C	1308	NAG	2	0
10	B	1305	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

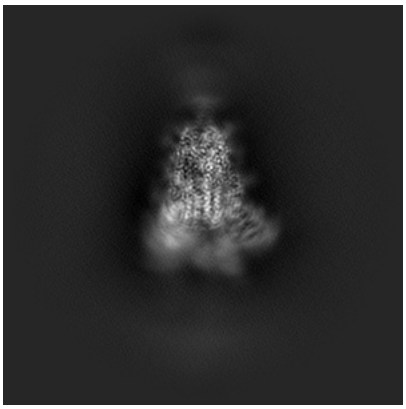
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27073. These allow visual inspection of the internal detail of the map and identification of artifacts.

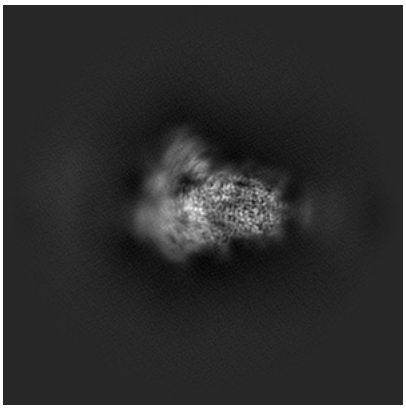
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

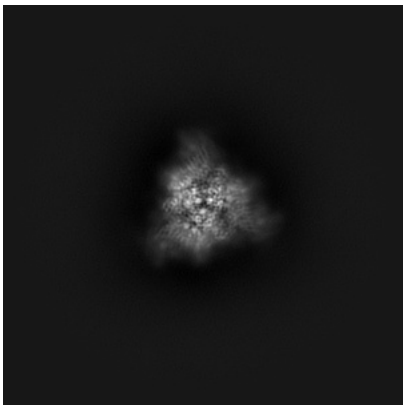
6.1.1 Primary map



X

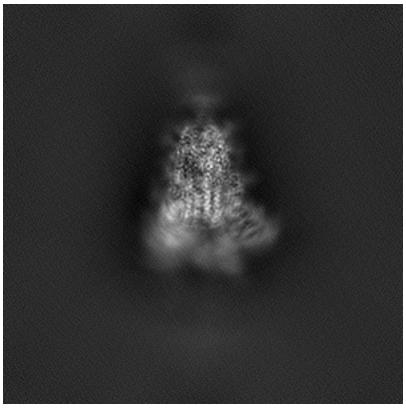


Y

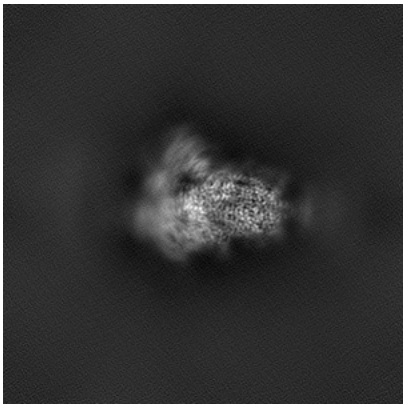


Z

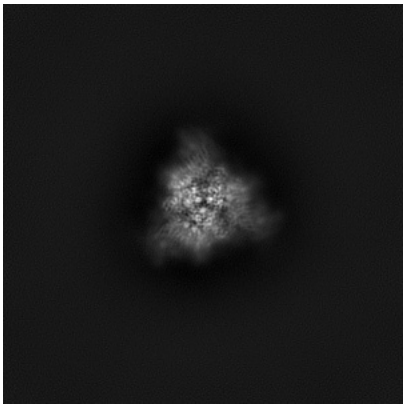
6.1.2 Raw map



X



Y

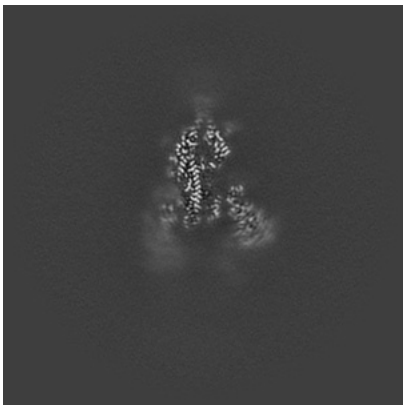


Z

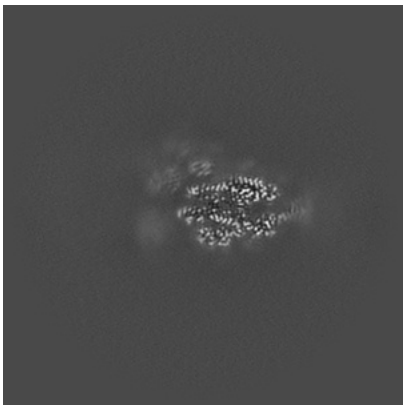
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

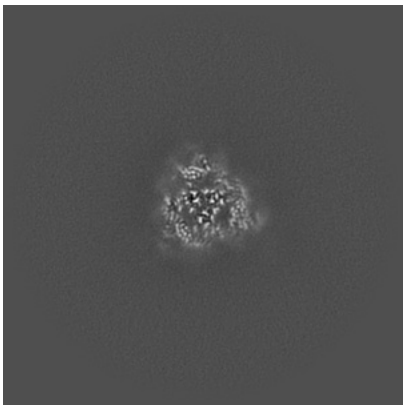
6.2.1 Primary map



X Index: 160

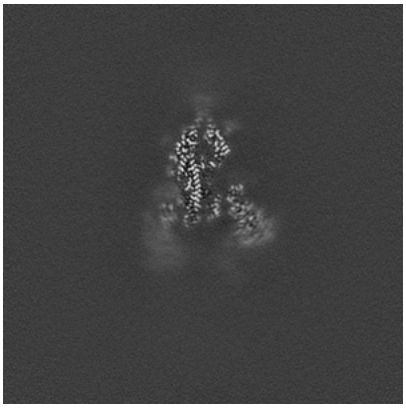


Y Index: 160

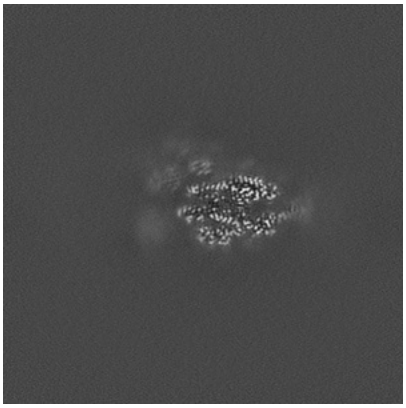


Z Index: 160

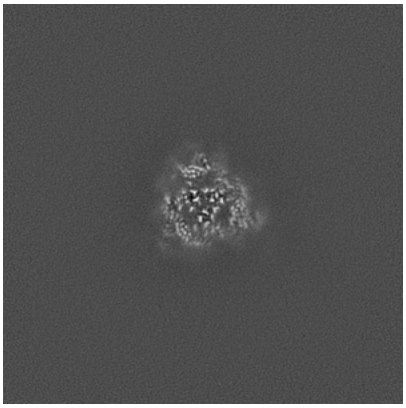
6.2.2 Raw map



X Index: 160



Y Index: 160

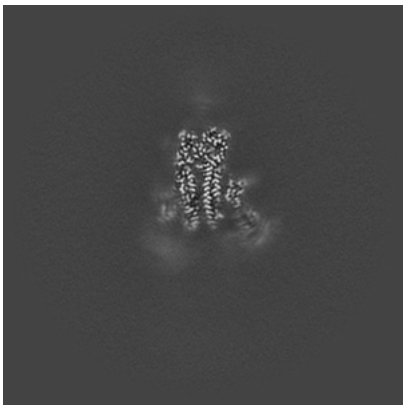


Z Index: 160

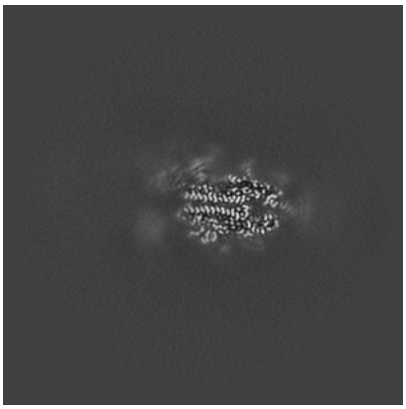
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

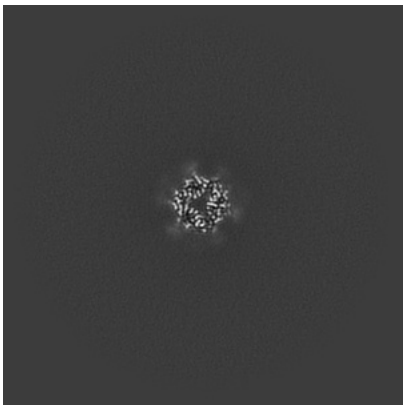
6.3.1 Primary map



X Index: 165

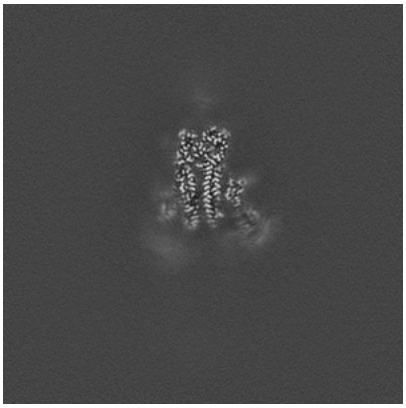


Y Index: 164

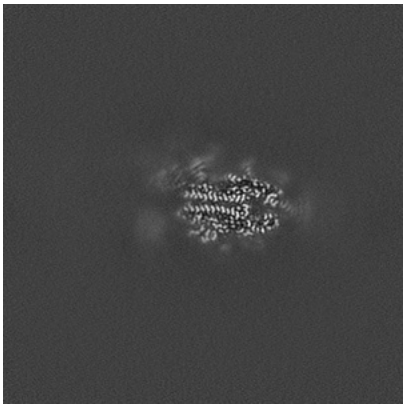


Z Index: 203

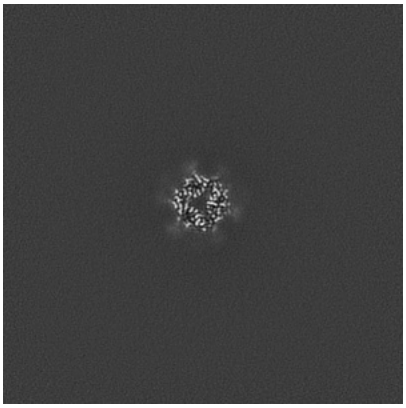
6.3.2 Raw map



X Index: 165



Y Index: 164



Z Index: 203

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

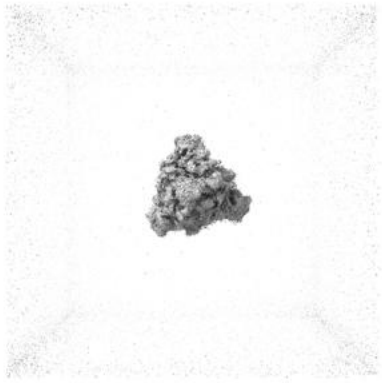
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X

Y



Z

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

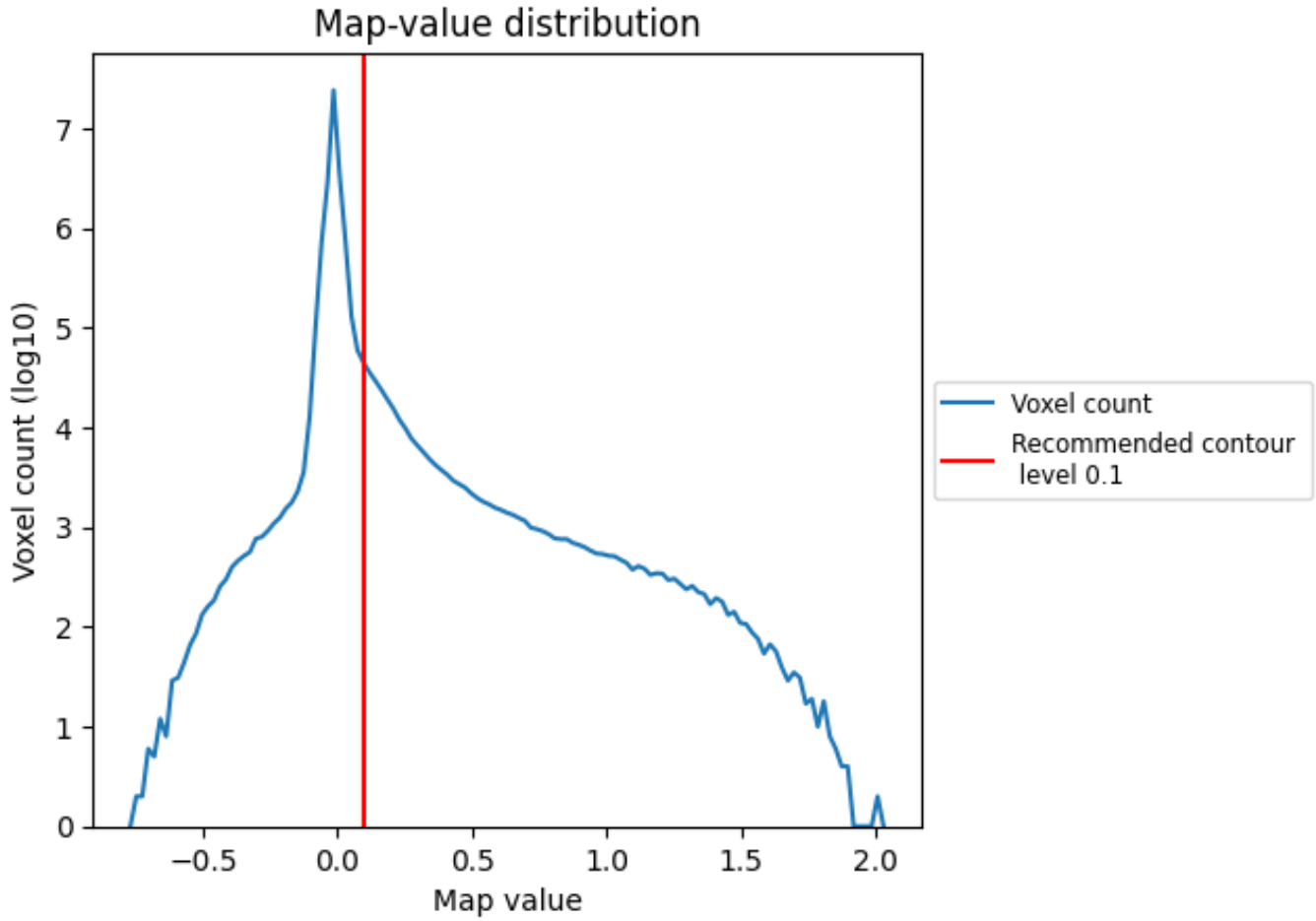
6.5 Mask visualisation (i)

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

7 Map analysis

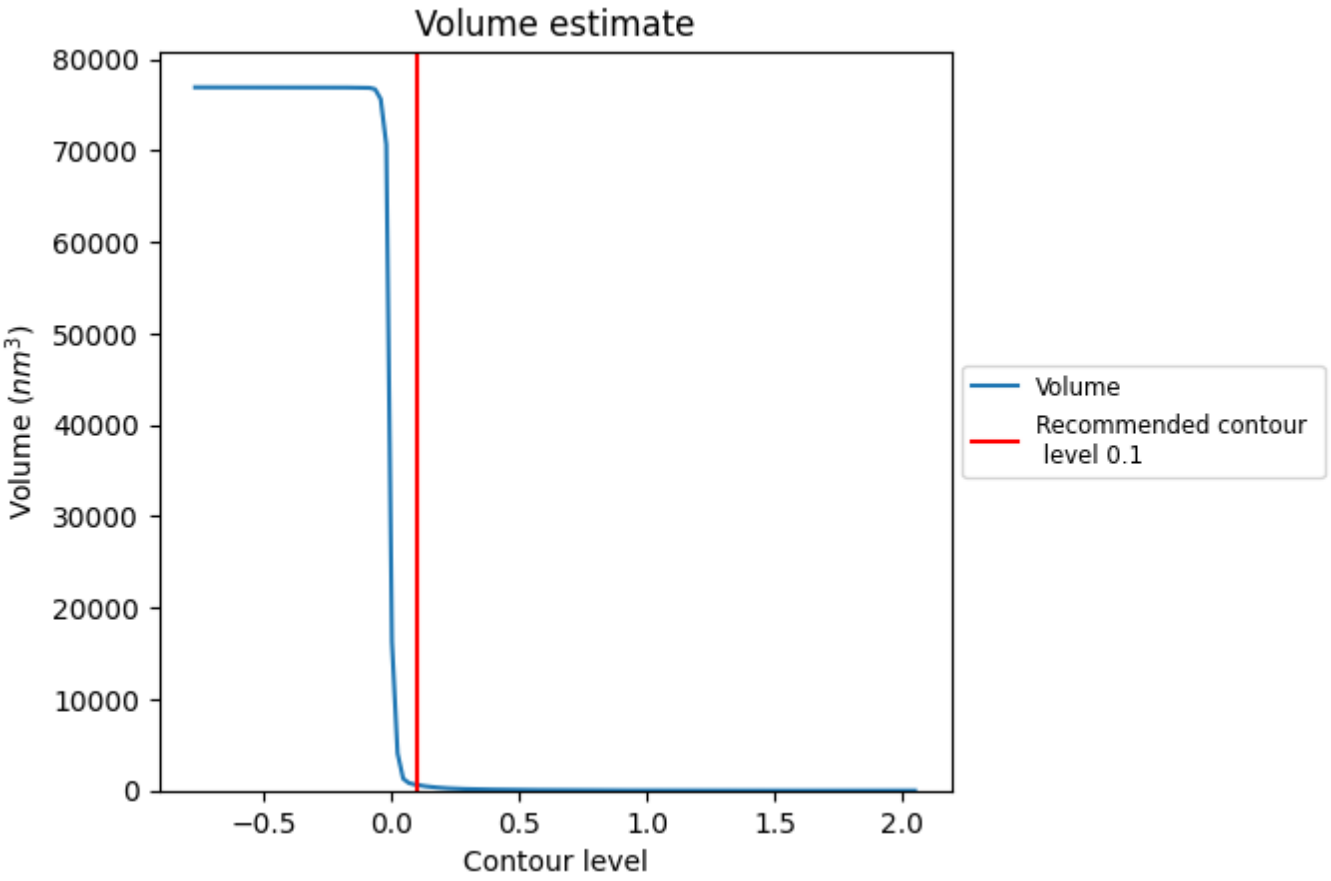
This section contains the results of statistical analysis of the map.

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.

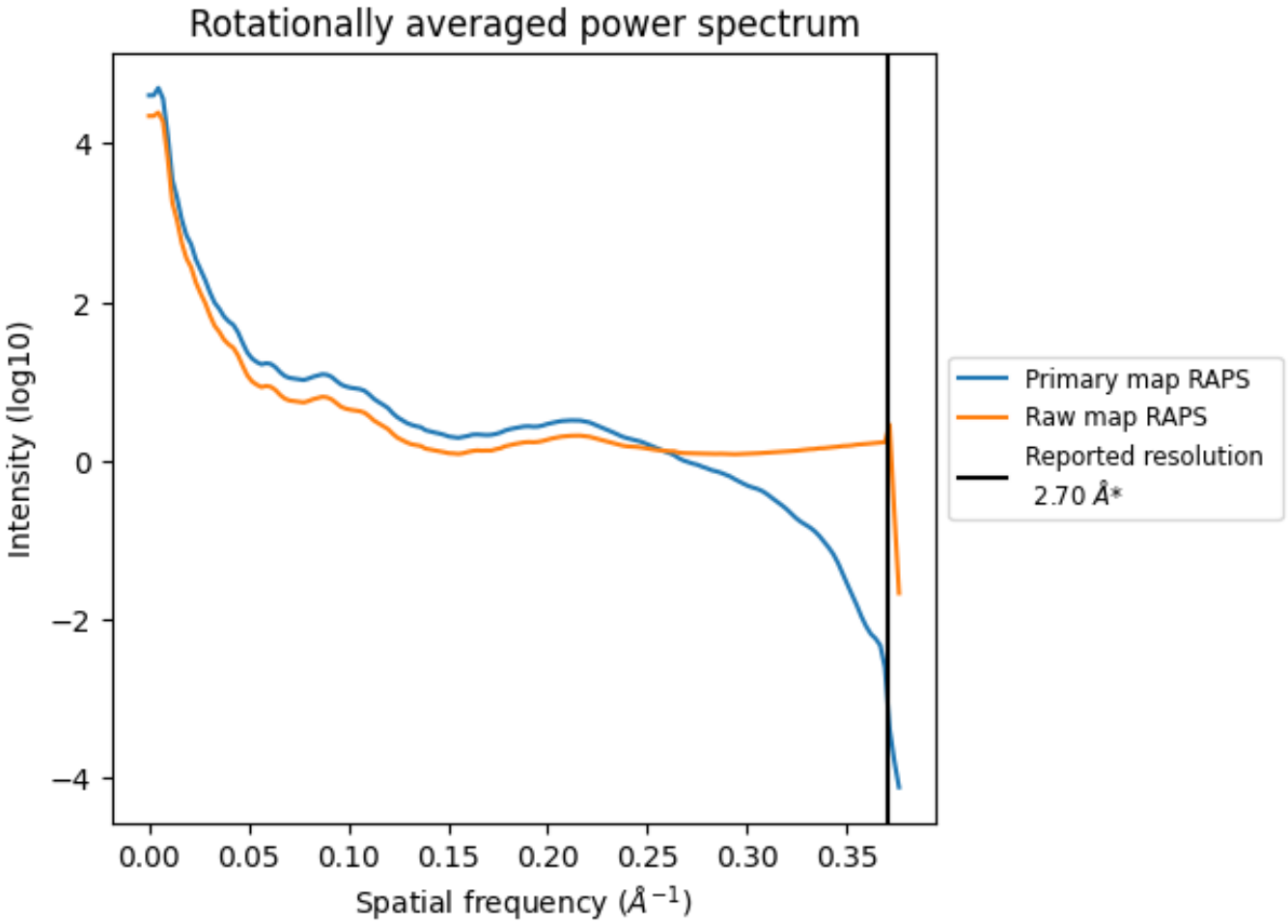
7.2 Volume estimate (i)



The volume at the recommended contour level is 614 nm^3; this corresponds to an approximate mass of 555 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)

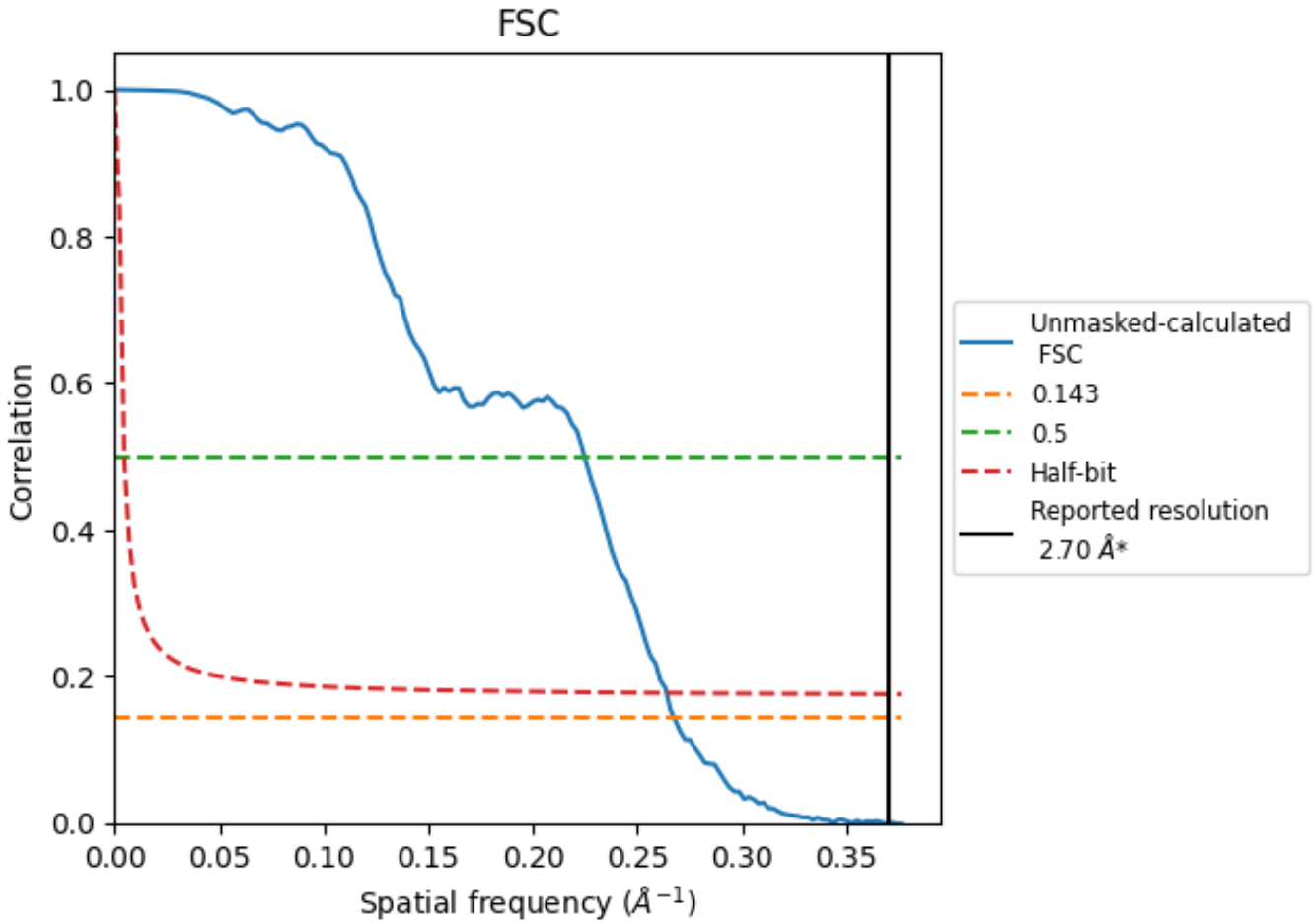


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

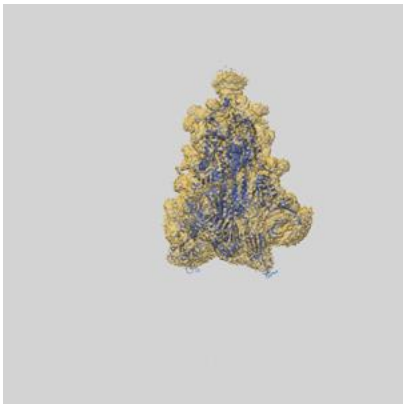
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.45	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.7 by more than 10 %

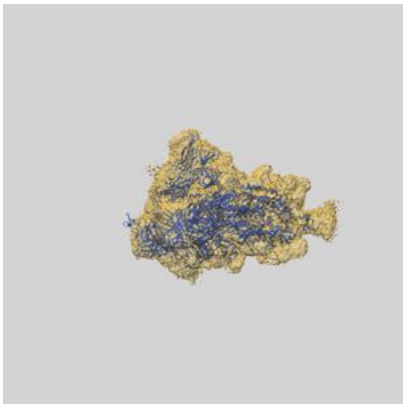
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27073 and PDB model 8CYB. Per-residue inclusion information can be found in section 3 on page 10.

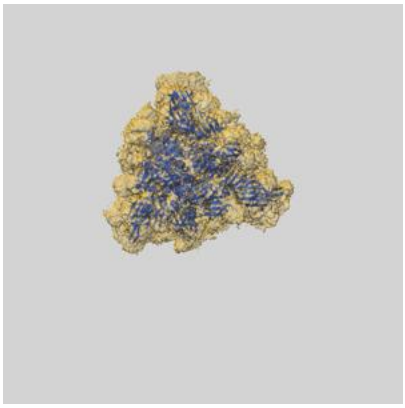
9.1 Map-model overlay



X



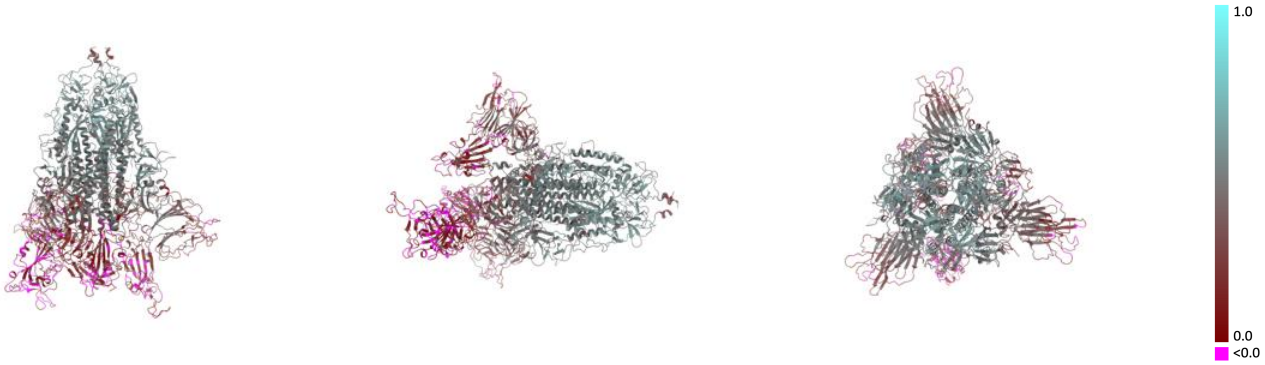
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

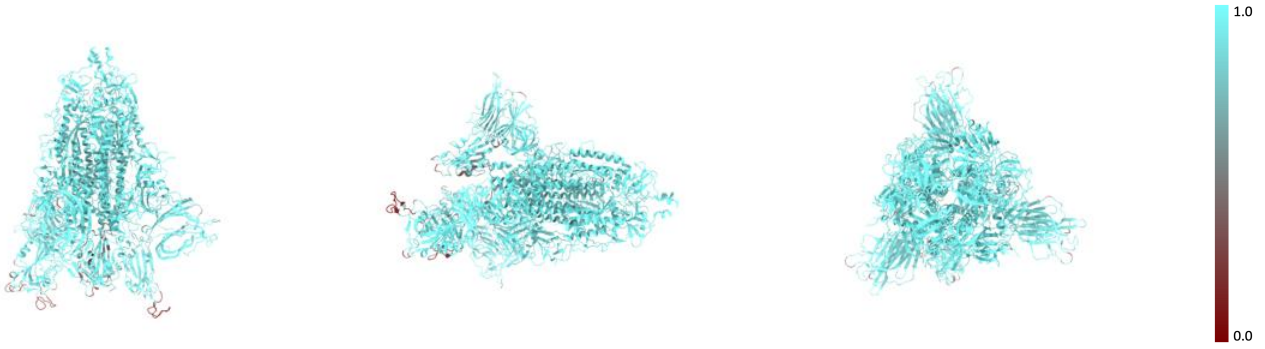
9.2 Q-score mapped to coordinate model (i)



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.

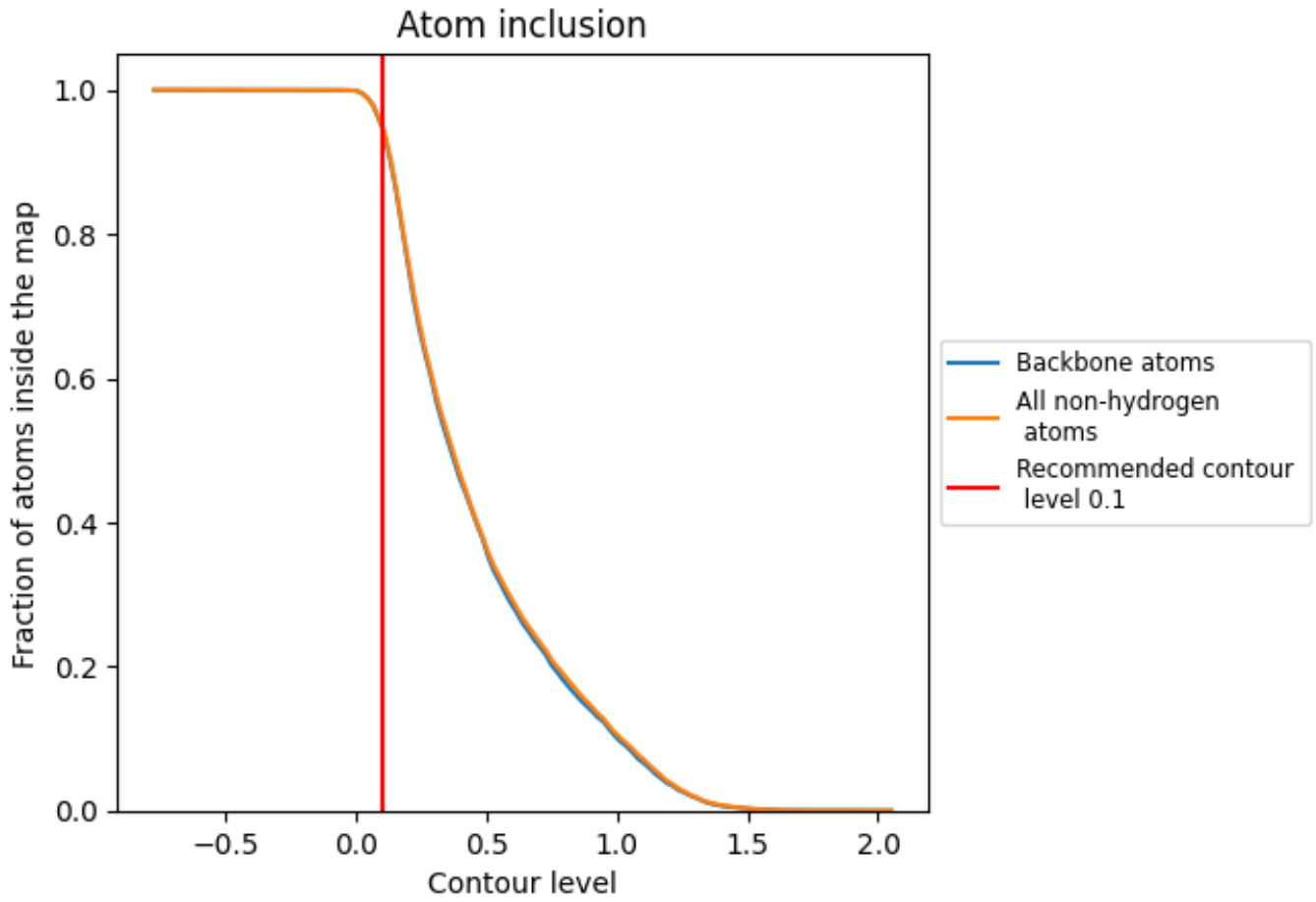
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9532	0.3530
A	0.9642	0.3730
B	0.9498	0.3430
C	0.9610	0.3780
D	0.7800	0.0340
E	1.0000	0.3710
F	1.0000	0.3650
G	1.0000	0.4770
H	1.0000	0.3150
I	0.9286	0.3230
J	1.0000	0.3600
K	1.0000	0.4300
L	1.0000	0.4330
M	1.0000	0.4140
N	0.9592	0.2450
O	1.0000	0.2950
P	1.0000	0.4800
Q	1.0000	0.3880
R	1.0000	0.2960
S	1.0000	0.3690
T	1.0000	0.3580
U	1.0000	0.3660
V	1.0000	0.3780
W	1.0000	0.4560
X	1.0000	0.2500
Y	1.0000	0.4650
Z	0.9744	0.3720