Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 07:13 PM JST

PDB ID	:	7CN9
EMDB ID	:	EMD-30419
Title	:	Cryo-EM structure of SARS-CoV-2 Spike ectodomain
Authors	:	Ho, M.; Chang, Y.; Wang, C.; Wu, Y.; Huang, H.; Chen, T.; Lo, J.M.; Chen, X.; Ma, C.
Deposited on	:	2020-07-30
Resolution	:	4.70 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 (i) 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 (i)) were used in the production of this report:

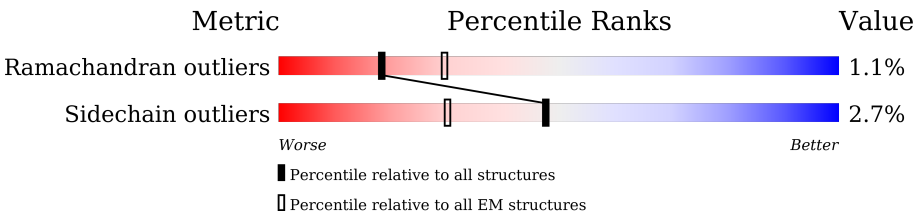
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

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 4.70 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)
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	1127	44% 87% • 10%
1	B	1127	37% 87% • 10%
1	C	1127	39% 89% • 8%
2	E	2	100% 50% 50%
2	H	2	50% 100%
2	N	2	100% 50% 50%
2	W	2	100%
2	X	2	50% 100%
2	Z	2	100% 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	d	2	50% 50% 50%
2	f	2	50% 50%
3	k	3	67% 33% 67%
4	V	3	67% 100%
4	p	3	33% 100%
5	h	4	100% 50% 50%
6	Q	4	75% 100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1011	7727	4935	1292	1465	35	0	0
1	B	1010	7674	4895	1285	1458	36	0	0
1	C	1037	7889	5040	1316	1498	35	0	0

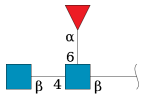
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	GLY	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	GLY	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

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

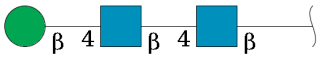
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	E	2	28	16	2	10	0	0
2	X	2	28	16	2	10	0	0
2	W	2	28	16	2	10	0	0
2	Z	2	28	16	2	10	0	0
2	d	2	28	16	2	10	0	0
2	f	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	N	2	28	16	2	10	0	0

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



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

- Molecule 4 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
			Total	C	N	O		
4	p	3	39	22	2	15	0	0
4	V	3	39	22	2	15	0	0

- Molecule 5 is an oligosaccharide called 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-gluco

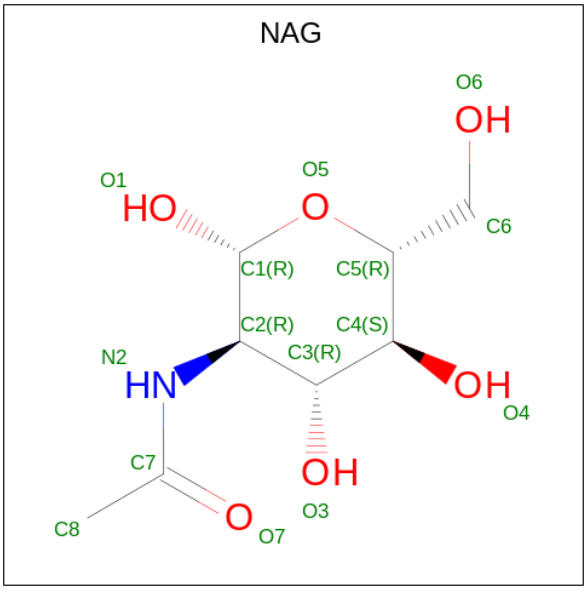
pyranose.

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

- Molecule 6 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
			Total	C	N	O		
6	Q	4	50	28	2	20	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	98	56	7	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	98	56	7	35	0
7	A	1	98	56	7	35	0
7	A	1	98	56	7	35	0
7	A	1	98	56	7	35	0
7	A	1	98	56	7	35	0
7	A	1	98	56	7	35	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	C	1	98	56	7	35	0
7	C	1	98	56	7	35	0
7	C	1	98	56	7	35	0
7	C	1	98	56	7	35	0
7	C	1	98	56	7	35	0
7	C	1	98	56	7	35	0

Continued on next page...

Continued from previous page...

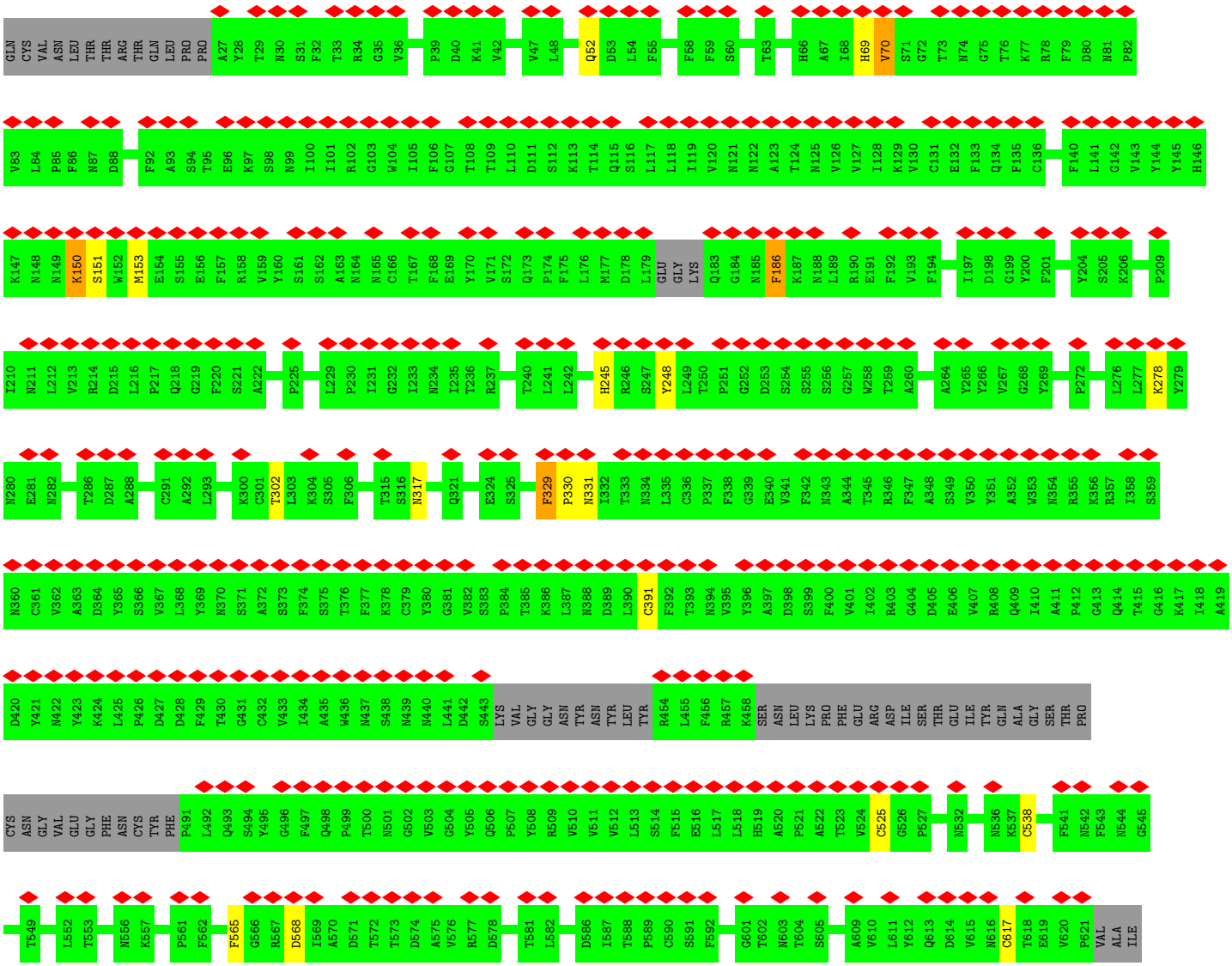
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	C	1	98	56	7	35	0

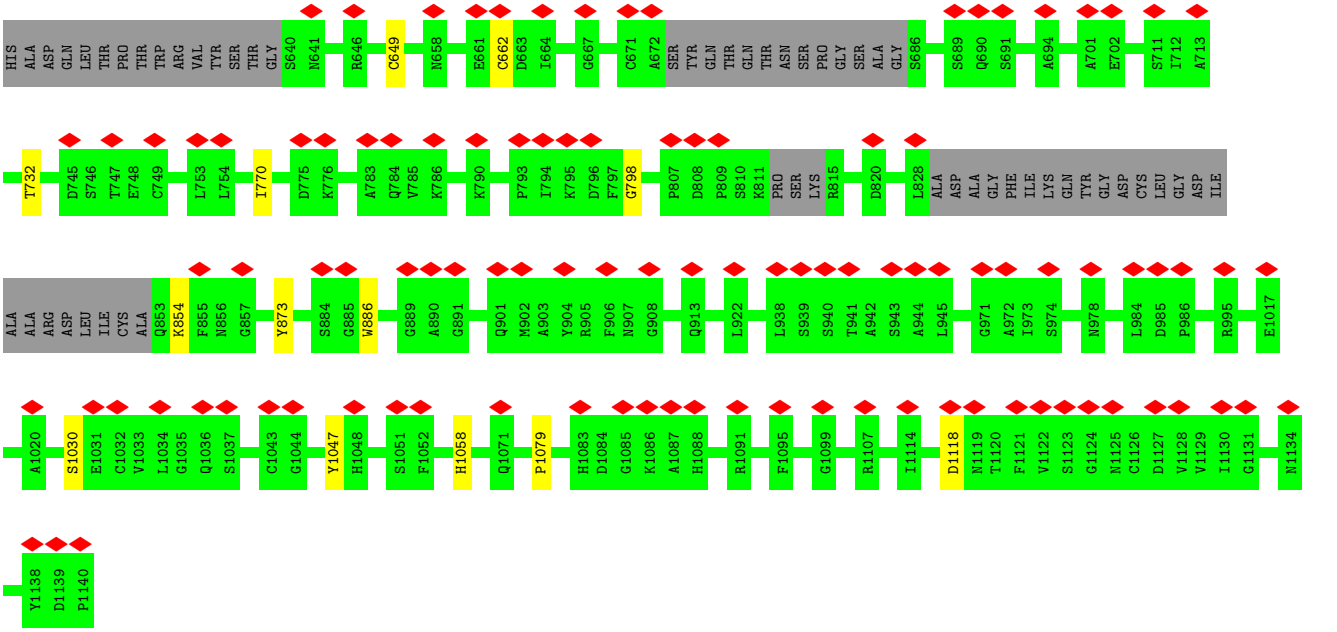
3 Residue-property plots (i)

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

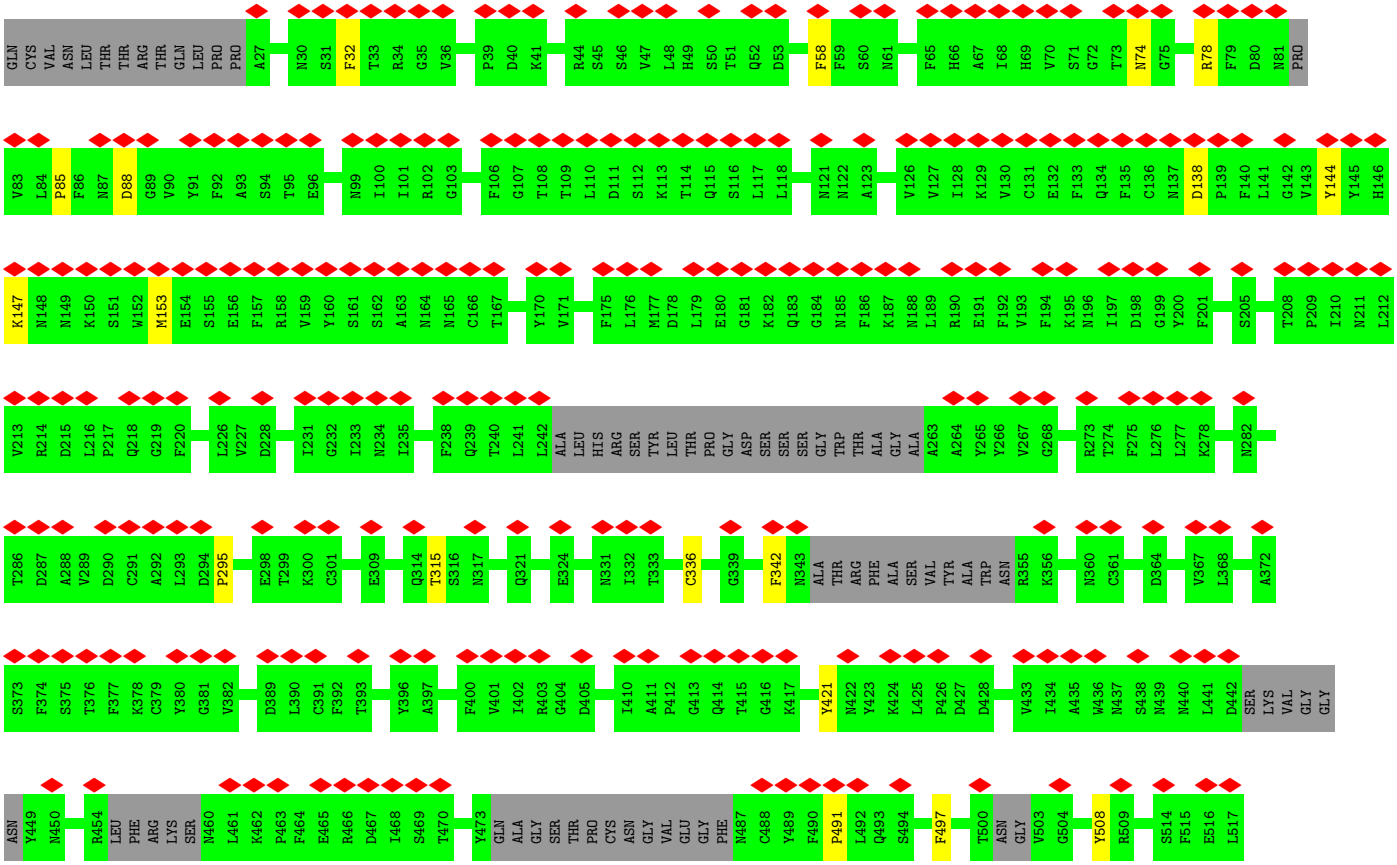
Chain A:





- Molecule 1: Spike glycoprotein

Chain B:



L518 H519 A520 P521 A522 C525 G526 P527 K537 C538 N542 G545 L546 T547 V551 L552 T553 E554 S555 N556 K557 K558 P561 T562 R567 D568 D571 T572 T573 D574 D586 I587 T588 P589 C590 S591 S596 N603 T604 S605 A609 V610 L611 Y612 Q613 D614 V615

T618 V622 A623 I624 H625 A626 D627 Q628 L629 THR PRO THR TRP ARG VAL TYR SER T638 G639 S640 N641 R646 C649 L650 E661 C662 D663 I664 G667 A672 SER TYR GLN THR GLN THR ASN SER PRO GLY SER ALA GLY SER V687 Q690 A694 E702 A706

N710 S711 I712 F715 I726 K733 D745 S746 T747 L753 L754 F759 L763 N764 R765 E780 V781 F782 A783 Q784 I794 K795 D796 G799 S803 D808 K811 P812 S813 K814 R815 D820 F823 N824 L828 ALA ASP ALA GLY PHE ILE LYS GLN TYR

GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA Q853 K854 F855 N856 G857 L864 M869 Y873 I882 T883 S884 G885 W886 T887 F888 G889 A890 G891 A892 Q895 I896 P897 M902 A903 Y904 R905 F906 T912 Q913 Y917 K921 S939 S940 T941 A942

S943 A944 K947 I973 N978 R983 E988 Q1002 E1017 T1027 E1031 C1032 Q1036 S1037 D1041 F1042 C1043 G1044 S1051 Q1071 T1077 A1078 P1079 D1084 G1085 K1086 A1087 R1091 E1092 G1093 G1099 R1107 T1117 D1118 S1123 G1124 N1125 C1126 D1127

I1130 G1131 I1132 V1133 N1134 N1135 T1136 V1137 Y1138 D1139 P1140

- Molecule 1: Spike glycoprotein

Chain C:

GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO A27 N30 S31 F32 T33 R34 G35 V36 P39 D40 K41 R44 V47 Q52 D53 L54 F55 S60 N61 V62 T63 H66 A67 I68 H69 V70 S71 G72 T73 N74 G75 T76 K77 R78 F79 D80 N81 P82 V83 L84

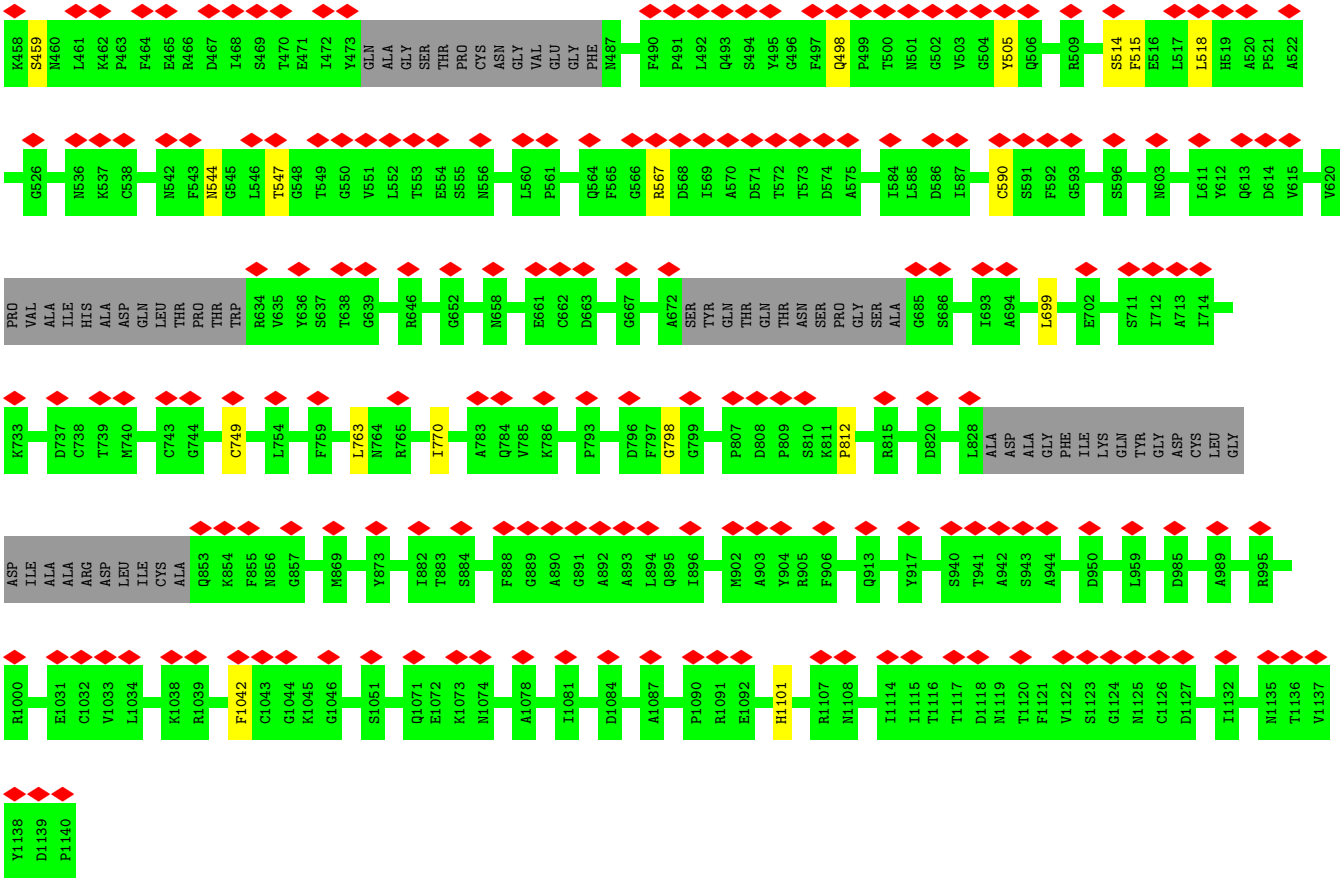
P85 D88 G89 V90 Y91 F92 A93 S94 T95 E96 K97 S98 N99 I100 I101 R102 G103 W104 I105 F106 G107 T108 T109 L110 D111 S112 K113 T114 Q115 S116 L117 L118 I119 V120 N121 N122 A123 V126 V127 I128 C131 E132 F133 Q134 F135 C136 N137 D138 P139 F140 L141 G142 V143 Y144 Y145 H146 K147

N148 N149 K150 S151 W152 M153 E154 S155 E156 F157 R158 V159 TYR SER SER ALA ASN N165 C166 T167 F168 E169 Y170 V171 S172 L176 MET ASP LEU GLU GLY LYS GLN GLY ASN PHE K187 E191 F192 V193 F194 K195 N196 I197 D198 G199 Y200 F201 K202 I203 K206 P209 I210 V213

P217 Q218 G219 F220 S221 A222 L223 L229 P230 I231 G232 I233 N234 I235 F238 Q239 T240 L241 L242 A243 L244 H245 R246 S247 Y248 L249 T250 P251 G252 D253 S254 S255 S256 T259 A262 A263 A264 V267 G268 Y269 L270 Q271 P272 R273 T274 F275 L276 L277 K278 Y279 N280 E281 T284 I285

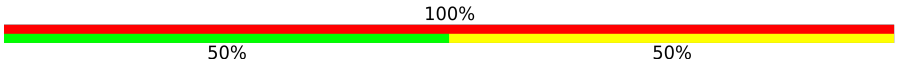
T286 D287 A288 C291 A292 E298 T299 K300 S316 N317 F318 R319 V320 Q321 E324 S325 F329 P330 N331 I332 T333 N334 L335 C336 P337 F338 G339 E340 T345 R346 Y351 A352 R355 K356 R357 I358 S359 N360 A363 D364 Y365 S366 V367 L368 Y369 N370 S371 A372 S373 F374 S375

T376 F377 L387 N388 D389 L390 C391 F392 Y396 S399 F400 V401 I402 R403 Q409 I410 A411 P412 T415 G416 K417 I418 A419 D420 Y423 K424 L425 P426 D427 D428 F429 T430 G431 A435 W436 N439 N440 L441 D442 S443 K444 V445 G446 G447 N448 Y449 Y453 R454 L455 F456 R457



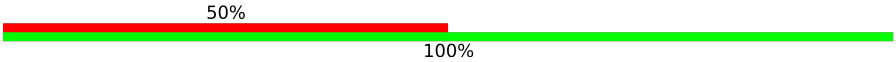
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



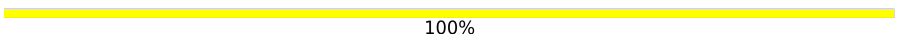
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

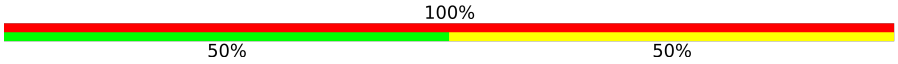


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



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

Chain Z: 

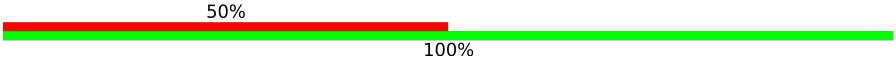
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

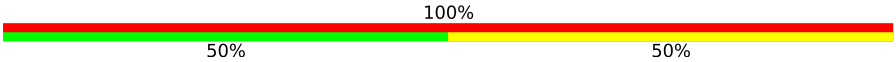
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

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

Chain H: 

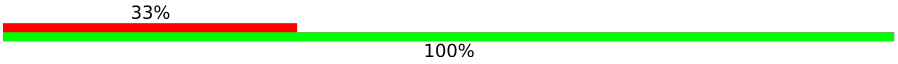
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

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

Chain k:

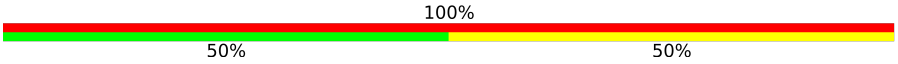
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

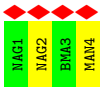
Chain p: 

• Molecule 4: 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-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 6: 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 Q:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00738	Depositor
Map size (Å)	354.24, 354.24, 354.24	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.55	2/7900 (0.0%)	0.63	1/10764 (0.0%)
1	B	0.54	0/7839	0.62	0/10679
1	C	0.57	2/8069 (0.0%)	0.62	1/11005 (0.0%)
All	All	0.55	4/23808 (0.0%)	0.62	2/32448 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	PRO	N-CA	13.68	1.70	1.47
1	C	330	PRO	N-CA	13.67	1.70	1.47
1	A	329	PHE	C-N	6.05	1.45	1.34
1	C	329	PHE	C-N	6.05	1.45	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	PRO	CA-N-CD	-9.52	98.17	111.50
1	C	330	PRO	CA-N-CD	-8.38	99.76	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	995/1127 (88%)	780 (78%)	205 (21%)	10 (1%)	15	54
1	B	988/1127 (88%)	770 (78%)	206 (21%)	12 (1%)	13	50
1	C	1023/1127 (91%)	780 (76%)	231 (23%)	12 (1%)	13	50
All	All	3006/3381 (89%)	2330 (78%)	642 (21%)	34 (1%)	18	52

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PHE
1	B	538	CYS
1	C	145	TYR
1	C	330	PRO
1	C	498	GLN
1	C	518	LEU
1	A	70	VAL
1	A	150	LYS
1	B	88	ASP
1	B	622	VAL
1	C	250	THR
1	C	252	GLY
1	C	454	ARG
1	A	617	CYS
1	B	78	ARG
1	B	85	PRO
1	A	69	HIS
1	A	151	SER
1	B	153	MET
1	B	295	PRO
1	A	186	PHE
1	A	1030	SER
1	B	74	ASN
1	B	605	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	783	ALA
1	B	823	PHE
1	C	749	CYS
1	C	812	PRO
1	C	247	SER
1	A	798	GLY
1	A	1079	PRO
1	C	798	GLY
1	B	491	PRO
1	C	272	PRO

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	838/976 (86%)	812 (97%)	26 (3%)	40	62
1	B	827/976 (85%)	809 (98%)	18 (2%)	52	71
1	C	850/976 (87%)	827 (97%)	23 (3%)	44	66
All	All	2515/2928 (86%)	2448 (97%)	67 (3%)	48	66

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	70	VAL
1	A	150	LYS
1	A	153	MET
1	A	186	PHE
1	A	245	HIS
1	A	248	TYR
1	A	278	LYS
1	A	302	THR
1	A	317	ASN
1	A	331	ASN
1	A	391	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	525	CYS
1	A	538	CYS
1	A	565	PHE
1	A	568	ASP
1	A	649	CYS
1	A	662	CYS
1	A	732	THR
1	A	770	ILE
1	A	854	LYS
1	A	873	TYR
1	A	886	TRP
1	A	1047	TYR
1	A	1058	HIS
1	A	1118	ASP
1	B	32	PHE
1	B	58	PHE
1	B	138	ASP
1	B	144	TYR
1	B	147	LYS
1	B	315	THR
1	B	336	CYS
1	B	342	PHE
1	B	421	TYR
1	B	497	PHE
1	B	508	TYR
1	B	763	LEU
1	B	811	LYS
1	B	813	SER
1	B	814	LYS
1	B	854	LYS
1	B	869	MET
1	B	1027	THR
1	C	44	ARG
1	C	122	ASN
1	C	145	TYR
1	C	253	ASP
1	C	331	ASN
1	C	334	ASN
1	C	355	ARG
1	C	403	ARG
1	C	455	LEU
1	C	457	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	459	SER
1	C	505	TYR
1	C	514	SER
1	C	515	PHE
1	C	544	ASN
1	C	547	THR
1	C	567	ARG
1	C	590	CYS
1	C	699	LEU
1	C	763	LEU
1	C	770	ILE
1	C	1042	PHE
1	C	1101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	87	ASN
1	A	99	ASN
1	A	125	ASN
1	A	134	GLN
1	A	146	HIS
1	A	148	ASN
1	A	207	HIS
1	A	613	GLN
1	A	641	ASN
1	A	655	HIS
1	A	658	ASN
1	A	751	ASN
1	A	777	ASN
1	A	787	GLN
1	A	901	GLN
1	A	920	GLN
1	A	928	ASN
1	A	935	GLN
1	A	949	GLN
1	A	953	ASN
1	A	969	ASN
1	A	1010	GLN
1	A	1048	HIS
1	A	1054	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1088	HIS
1	A	1108	ASN
1	B	49	HIS
1	B	87	ASN
1	B	121	ASN
1	B	185	ASN
1	B	388	ASN
1	B	506	GLN
1	B	542	ASN
1	B	564	GLN
1	B	607	GLN
1	B	655	HIS
1	B	764	ASN
1	B	784	GLN
1	B	953	ASN
1	B	954	GLN
1	B	992	GLN
1	B	1048	HIS
1	B	1071	GLN
1	B	1083	HIS
1	B	1101	HIS
1	B	1113	GLN
1	C	49	HIS
1	C	66	HIS
1	C	146	HIS
1	C	188	ASN
1	C	207	HIS
1	C	245	HIS
1	C	280	ASN
1	C	460	ASN
1	C	506	GLN
1	C	644	GLN
1	C	804	GLN
1	C	965	GLN
1	C	978	ASN
1	C	992	GLN
1	C	1048	HIS
1	C	1108	ASN
1	C	1135	ASN

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)

33 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.42	0	17,19,21	0.49	0
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	1.24	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.49	0	17,19,21	0.53	0
2	NAG	H	2	2	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	N	1	2,1	14,14,15	0.62	0	17,19,21	1.10	1 (5%)
2	NAG	N	2	2	14,14,15	0.40	0	17,19,21	0.36	0
6	NAG	Q	1	6,1	14,14,15	1.76	1 (7%)	17,19,21	1.54	3 (17%)
6	NAG	Q	2	6	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
6	BMA	Q	3	6	11,11,12	0.85	1 (9%)	15,15,17	0.96	1 (6%)
6	MAN	Q	4	6	11,11,12	0.96	1 (9%)	15,15,17	1.66	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.68	0
4	BMA	V	3	4	11,11,12	0.24	0	15,15,17	0.86	0
2	NAG	W	1	2,1	14,14,15	0.75	1 (7%)	17,19,21	0.73	0
2	NAG	W	2	2	14,14,15	0.85	2 (14%)	17,19,21	0.73	0
2	NAG	X	1	2,1	14,14,15	0.29	0	17,19,21	0.65	0
2	NAG	X	2	2	14,14,15	0.31	0	17,19,21	0.63	0
2	NAG	Z	1	2,1	14,14,15	0.61	1 (7%)	17,19,21	0.46	0
2	NAG	Z	2	2	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	d	1	2,1	14,14,15	0.52	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	d	2	2	14,14,15	0.16	0	17,19,21	0.85	1 (5%)
2	NAG	f	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	0.48	0
2	NAG	f	2	2	14,14,15	0.35	0	17,19,21	0.50	0
5	NAG	h	1	1,5	14,14,15	0.36	0	17,19,21	0.74	0
5	NAG	h	2	5	14,14,15	0.25	0	17,19,21	0.82	1 (5%)
5	BMA	h	3	5	11,11,12	0.74	0	15,15,17	0.85	0
5	MAN	h	4	5	11,11,12	0.82	1 (9%)	15,15,17	1.39	3 (20%)
3	NAG	k	1	3,1	14,14,15	0.32	0	17,19,21	0.54	0
3	NAG	k	2	3	14,14,15	0.42	0	17,19,21	0.99	1 (5%)
3	FUC	k	3	3	10,10,11	0.88	0	14,14,16	1.80	2 (14%)
4	NAG	p	1	4,1	14,14,15	0.37	0	17,19,21	0.78	0
4	NAG	p	2	4	14,14,15	0.33	0	17,19,21	0.66	0
4	BMA	p	3	4	11,11,12	0.27	0	15,15,17	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	3/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
2	NAG	W	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	X	2	2	-	5/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Z	2	2	-	3/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	4/6/23/26	0/1/1/1
5	NAG	h	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	h	2	5	-	1/6/23/26	0/1/1/1
5	BMA	h	3	5	-	0/2/19/22	0/1/1/1
5	MAN	h	4	5	-	1/2/19/22	0/1/1/1
3	NAG	k	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	k	2	3	-	3/6/23/26	0/1/1/1
3	FUC	k	3	3	-	-	0/1/1/1
4	NAG	p	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	p	2	4	-	5/6/23/26	0/1/1/1
4	BMA	p	3	4	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	1	NAG	O5-C1	-6.50	1.33	1.43
2	W	1	NAG	O5-C1	-2.75	1.39	1.43
5	h	4	MAN	C1-C2	2.31	1.57	1.52
2	Z	1	NAG	O5-C1	-2.19	1.40	1.43
2	W	2	NAG	C1-C2	2.15	1.55	1.52
6	Q	3	BMA	O3-C3	-2.09	1.38	1.43
2	f	1	NAG	O5-C1	-2.09	1.40	1.43
2	W	2	NAG	O5-C1	-2.08	1.40	1.43
6	Q	4	MAN	C1-C2	-2.05	1.47	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	4	MAN	C1-O5-C5	4.68	118.53	112.19
6	Q	1	NAG	C2-N2-C7	4.30	129.03	122.90
2	E	2	NAG	C2-N2-C7	4.19	128.87	122.90
3	k	3	FUC	C1-O5-C5	4.01	121.87	112.78
3	k	3	FUC	O5-C5-C4	3.88	116.48	109.52
3	k	2	NAG	C1-O5-C5	3.11	116.41	112.19
2	N	1	NAG	C1-O5-C5	3.04	116.31	112.19
6	Q	4	MAN	C1-C2-C3	-2.78	106.25	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	2	NAG	C1-O5-C5	2.76	115.93	112.19
5	h	4	MAN	C1-O5-C5	2.76	115.93	112.19
5	h	4	MAN	O2-C2-C3	-2.65	104.83	110.14
6	Q	1	NAG	C1-O5-C5	-2.43	108.90	112.19
6	Q	2	NAG	C1-O5-C5	2.34	115.36	112.19
5	h	2	NAG	C1-O5-C5	2.32	115.34	112.19
5	h	4	MAN	C1-C2-C3	2.24	112.42	109.67
6	Q	3	BMA	C3-C4-C5	-2.19	106.33	110.24
6	Q	1	NAG	O4-C4-C5	-2.18	103.88	109.30

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	1	NAG	C3-C2-N2-C7
2	X	1	NAG	O7-C7-N2-C2
4	p	2	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
2	X	1	NAG	C8-C7-N2-C2
4	p	1	NAG	C8-C7-N2-C2
4	p	1	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	W	2	NAG	C1-C2-N2-C7
4	p	3	BMA	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
4	p	3	BMA	C4-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	d	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	p	1	NAG	C1-C2-N2-C7
3	k	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	X	2	NAG	C8-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
2	N	2	NAG	O5-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	X	2	NAG	O7-C7-N2-C2
2	d	2	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C1-C2-N2-C7
5	h	4	MAN	O5-C5-C6-O6
3	k	1	NAG	C1-C2-N2-C7
5	h	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	X	2	NAG	C3-C2-N2-C7
3	k	2	NAG	C4-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
4	p	2	NAG	C4-C5-C6-O6
4	p	2	NAG	C8-C7-N2-C2
4	p	2	NAG	O5-C5-C6-O6
2	Z	1	NAG	C1-C2-N2-C7
2	Z	2	NAG	C1-C2-N2-C7
2	W	1	NAG	C3-C2-N2-C7
2	W	2	NAG	C3-C2-N2-C7
2	d	1	NAG	C3-C2-N2-C7
3	k	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

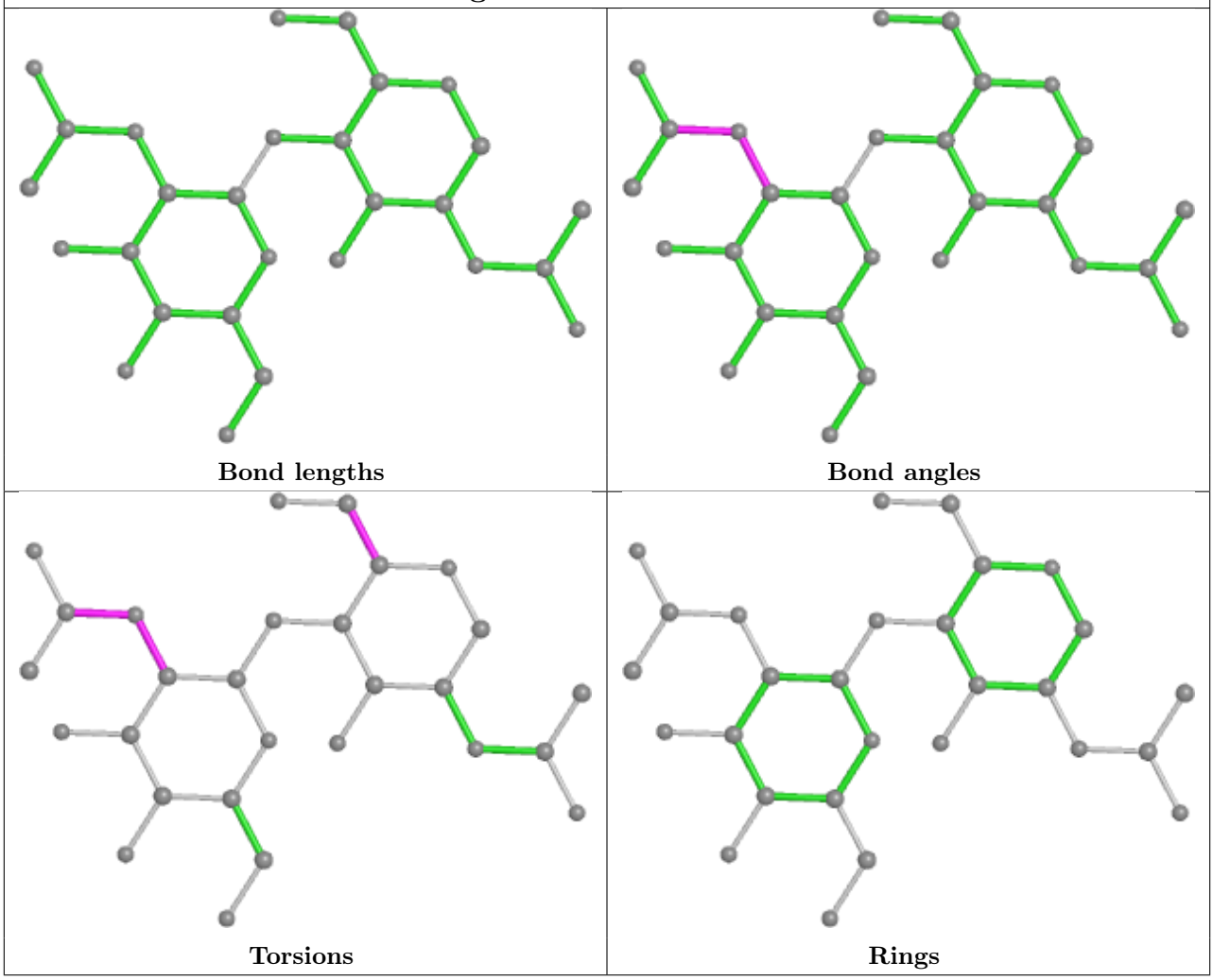
Mol	Chain	Res	Type	Atoms
6	Q	1	NAG	C3-C2-N2-C7
6	Q	2	NAG	C3-C2-N2-C7
4	p	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
3	k	1	NAG	C3-C2-N2-C7

There are no ring outliers.

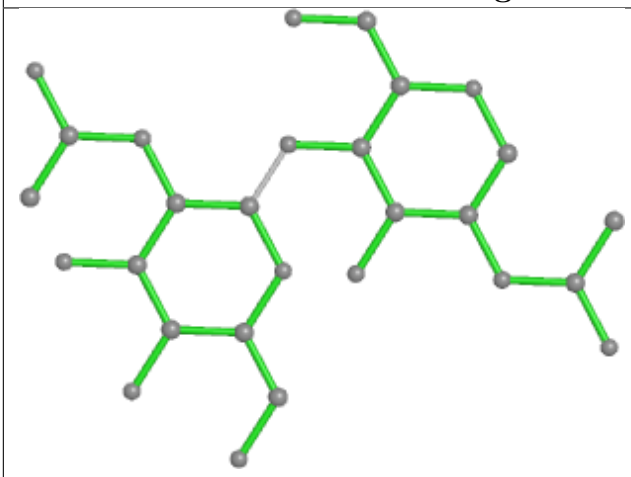
No monomer is involved in short contacts.

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

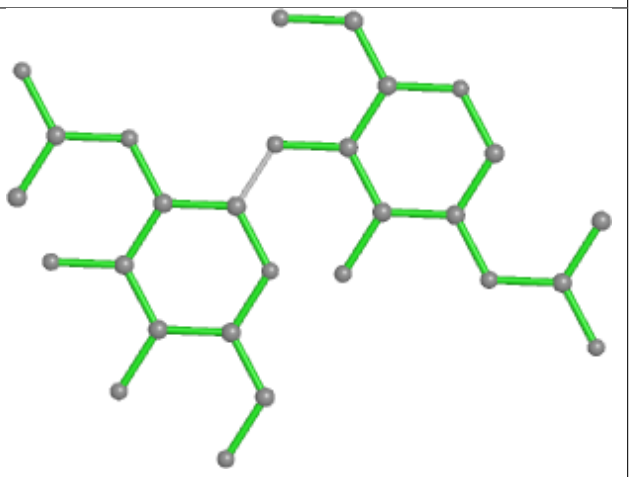
Oligosaccharide Chain E



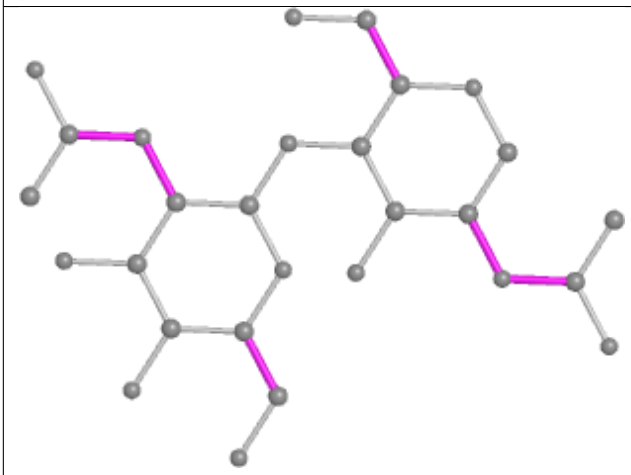
Oligosaccharide Chain X



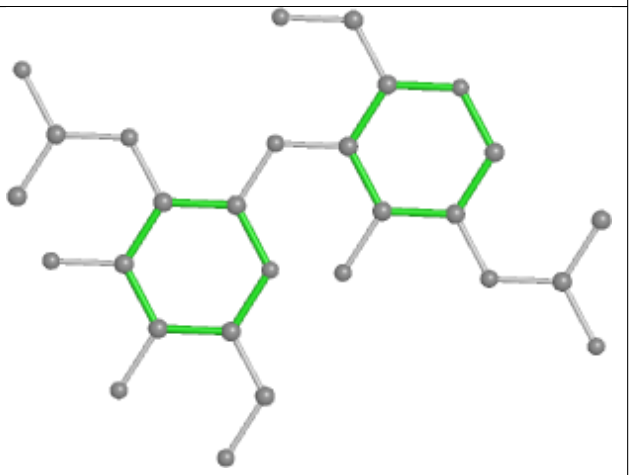
Bond lengths



Bond angles

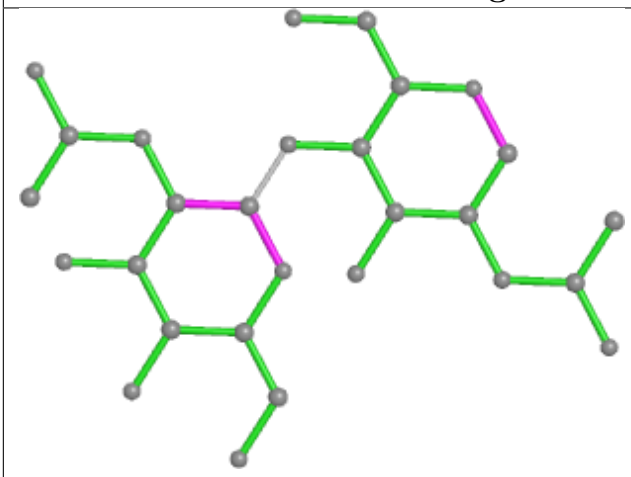


Torsions

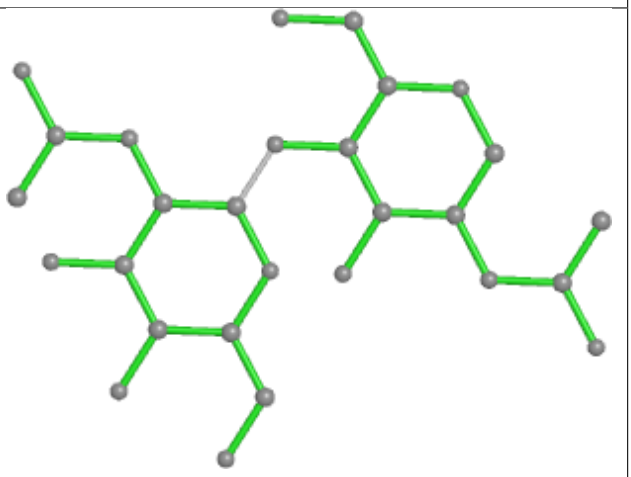


Rings

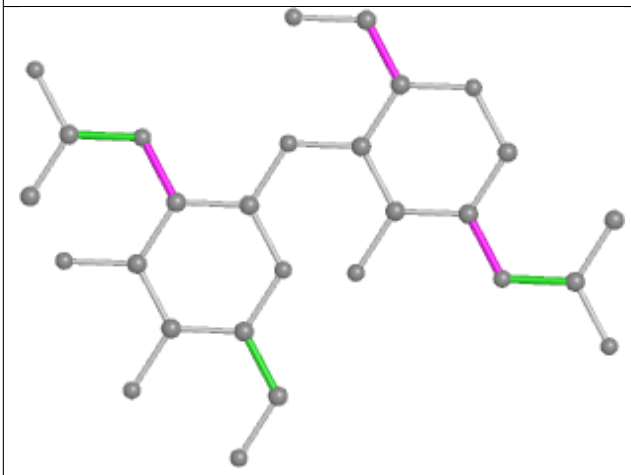
Oligosaccharide Chain W



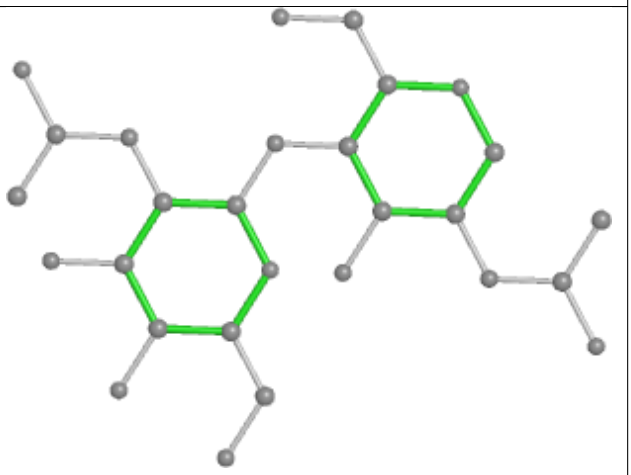
Bond lengths



Bond angles

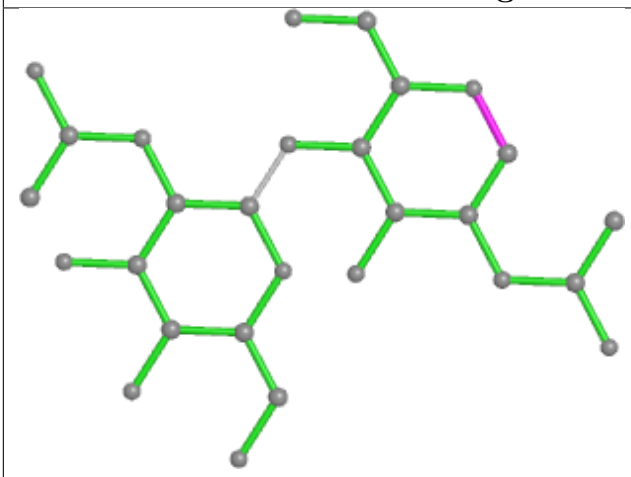


Torsions

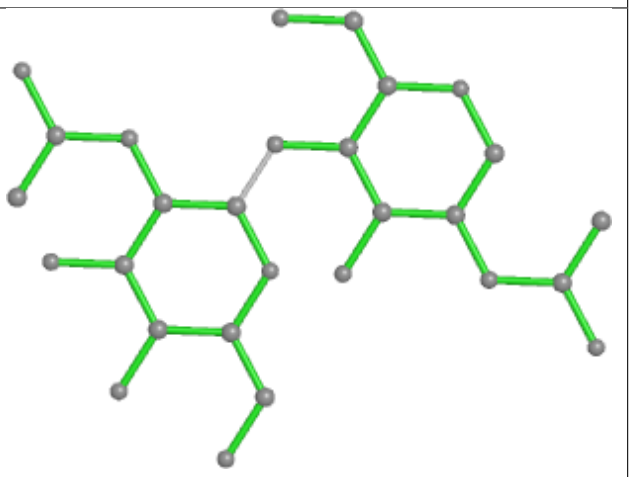


Rings

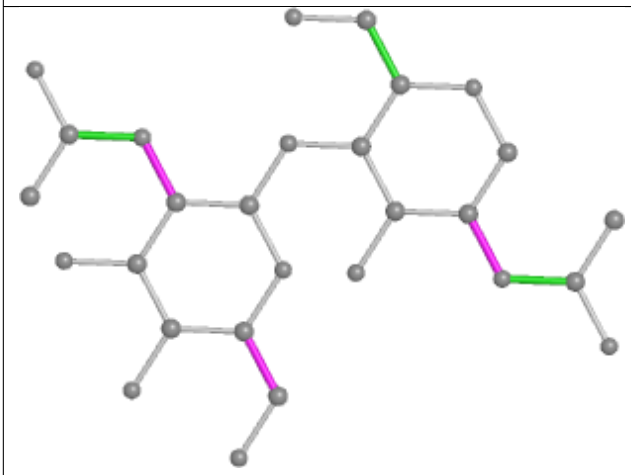
Oligosaccharide Chain Z



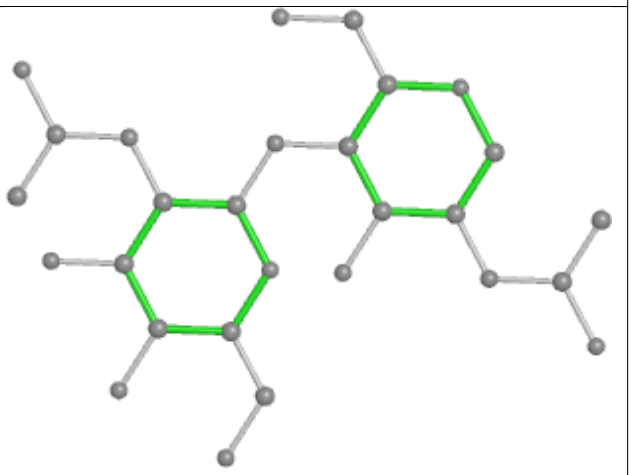
Bond lengths



Bond angles

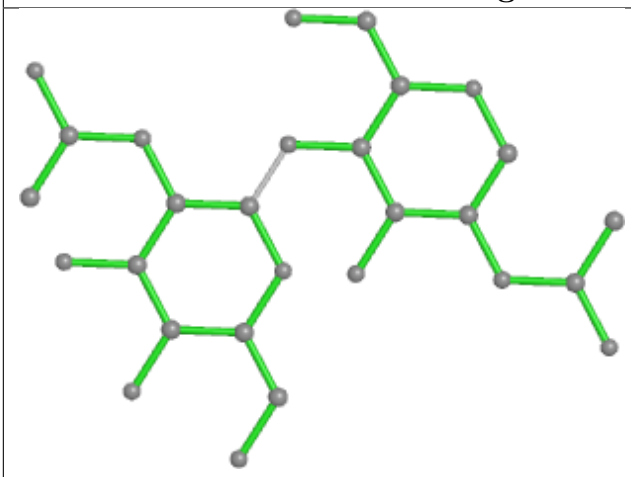


Torsions

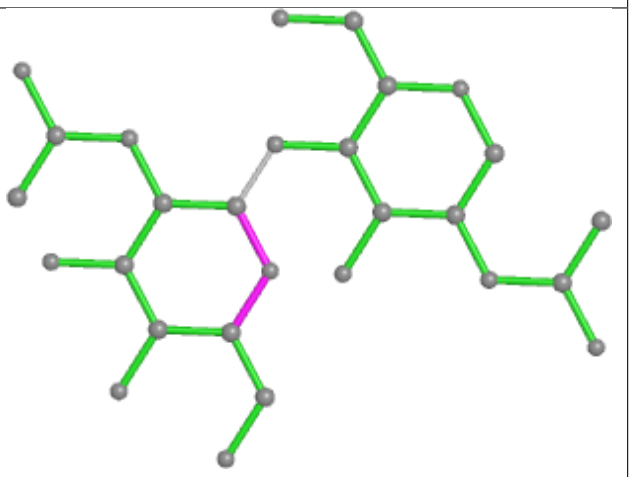


Rings

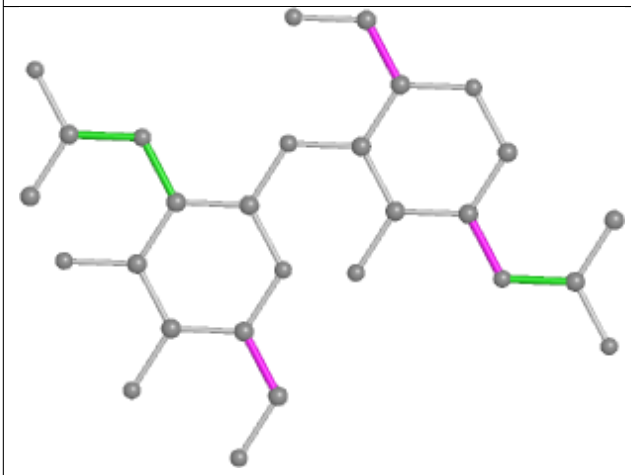
Oligosaccharide Chain d



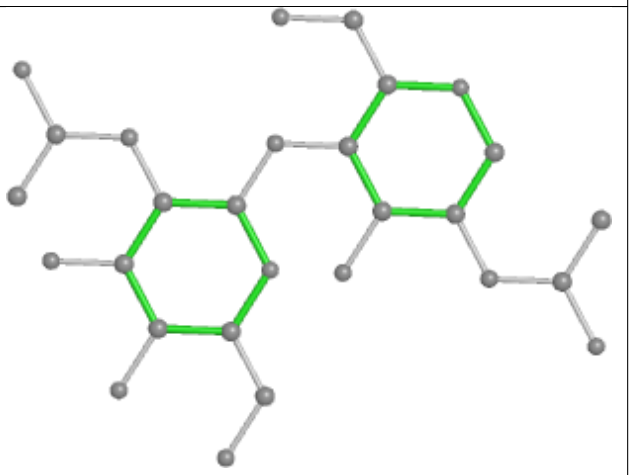
Bond lengths



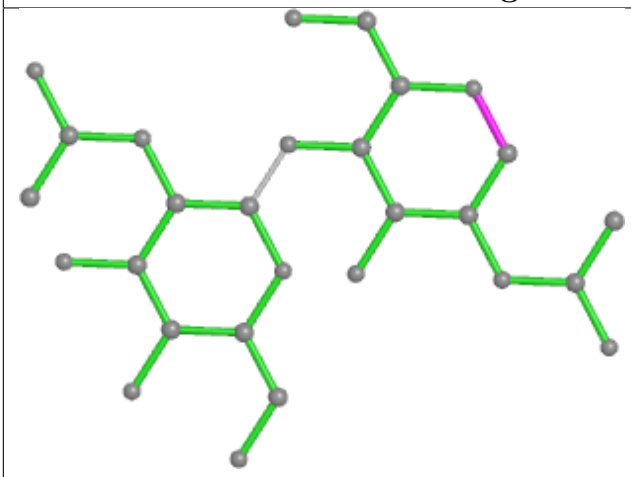
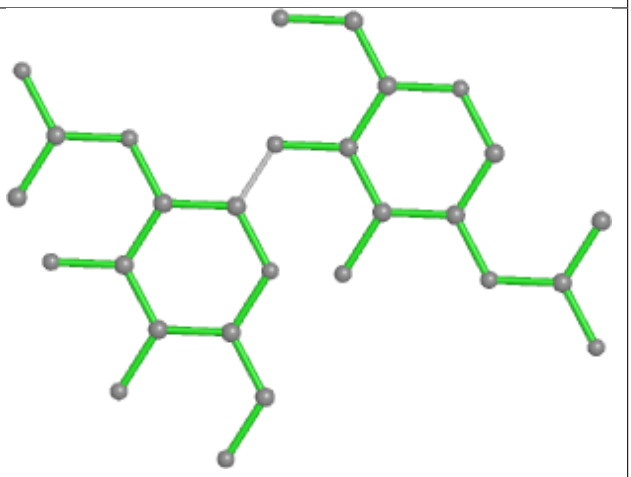
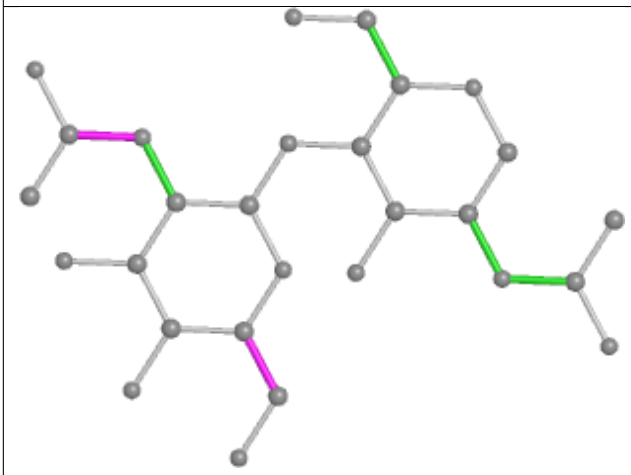
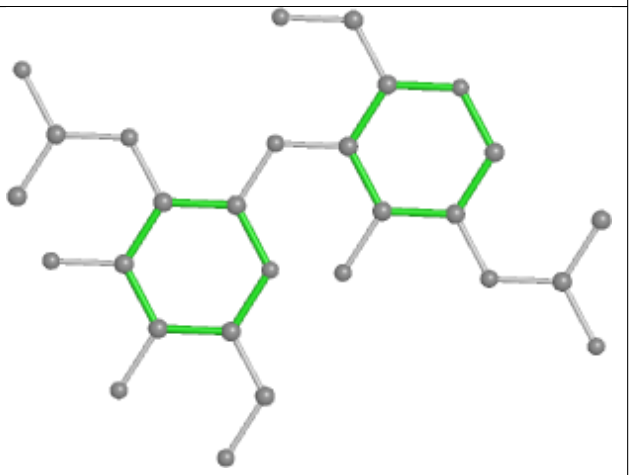
Bond angles

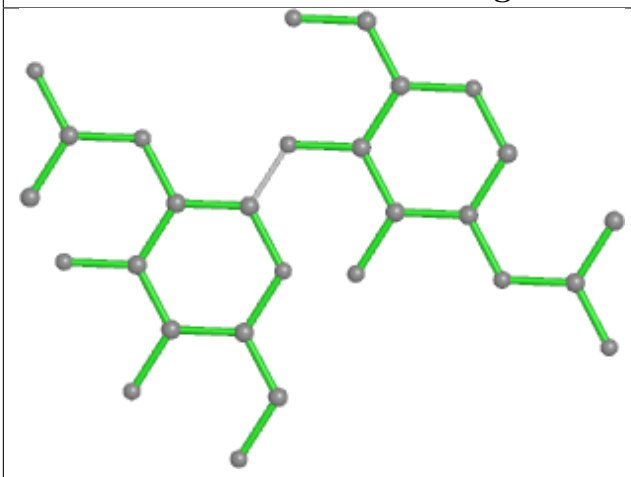
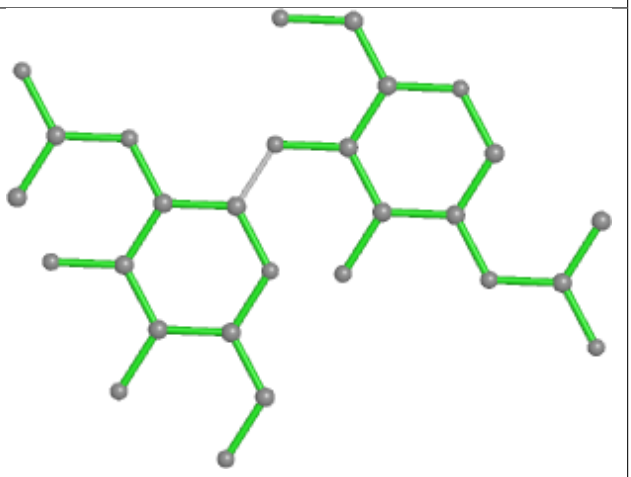
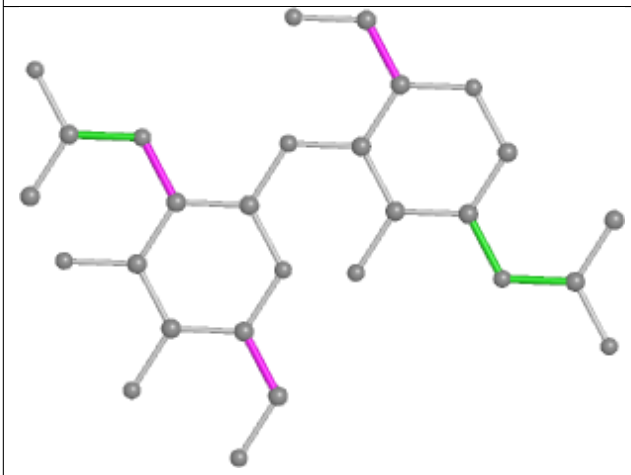
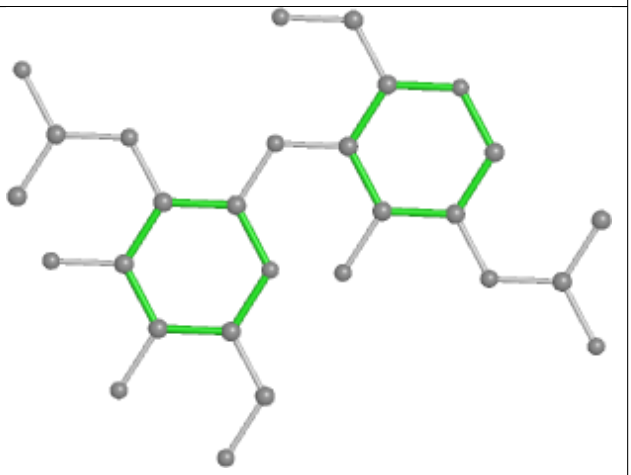


Torsions

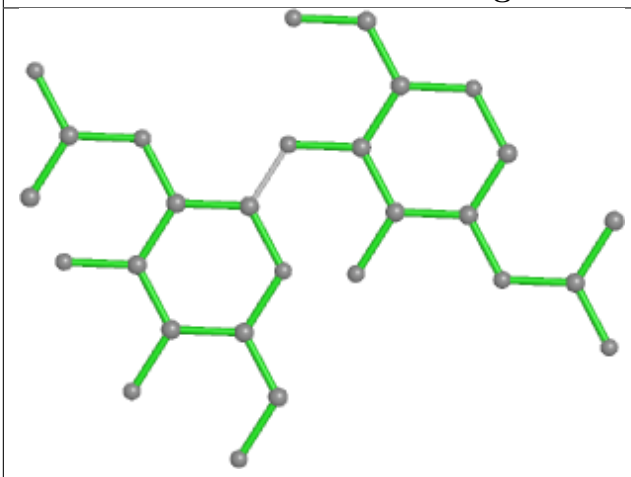


Rings

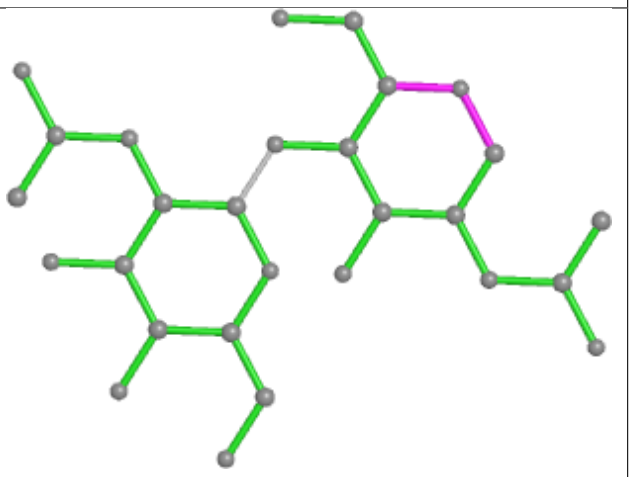
Oligosaccharide Chain f	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

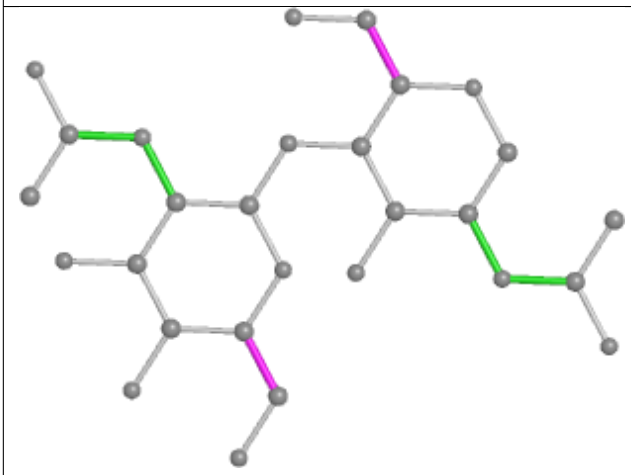
Oligosaccharide Chain N



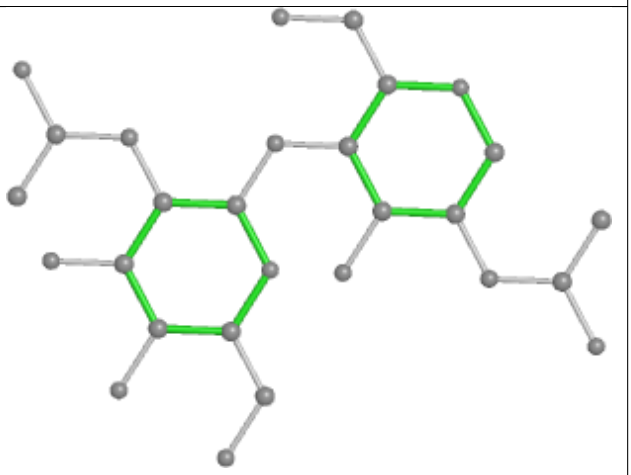
Bond lengths



Bond angles

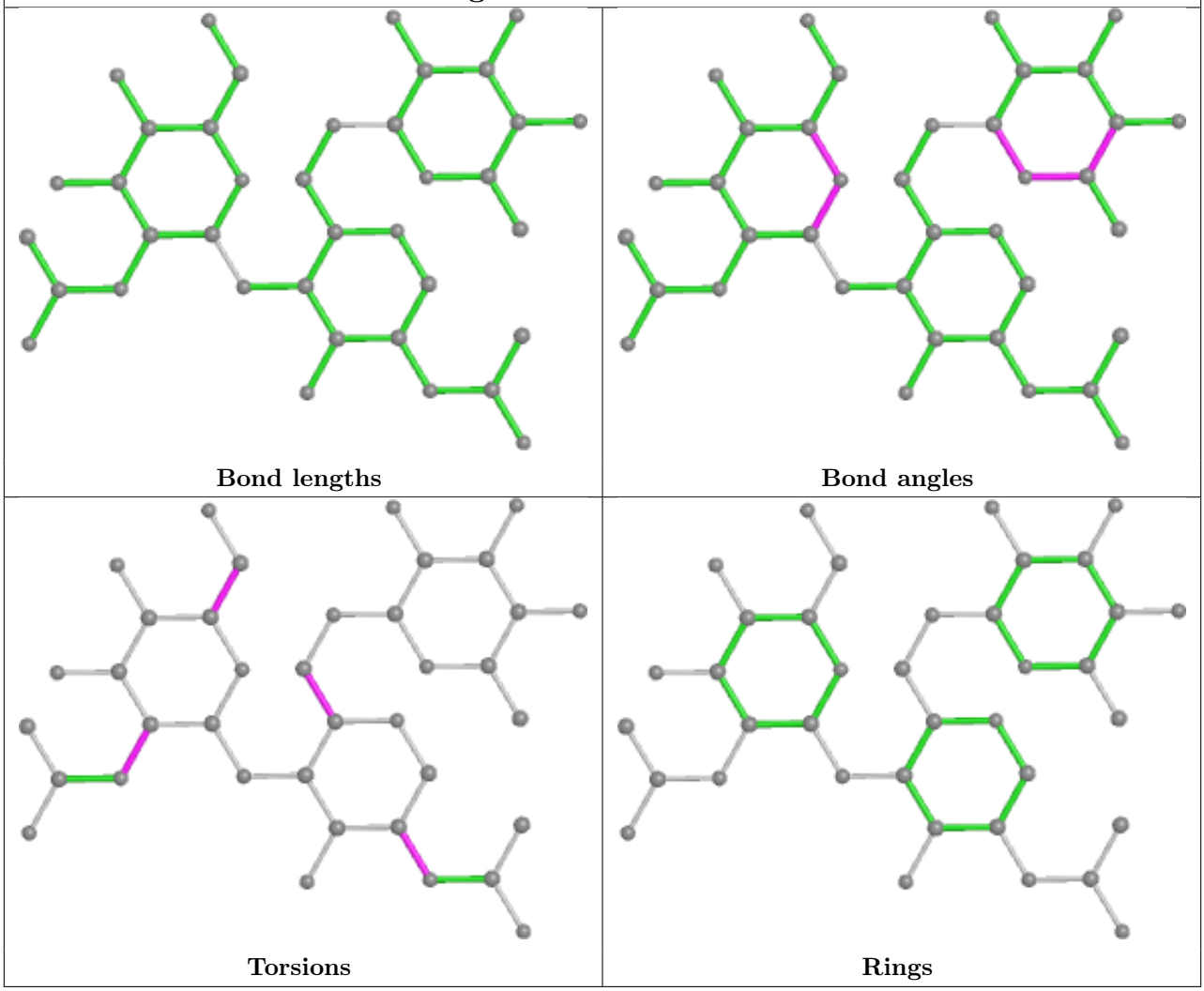


Torsions

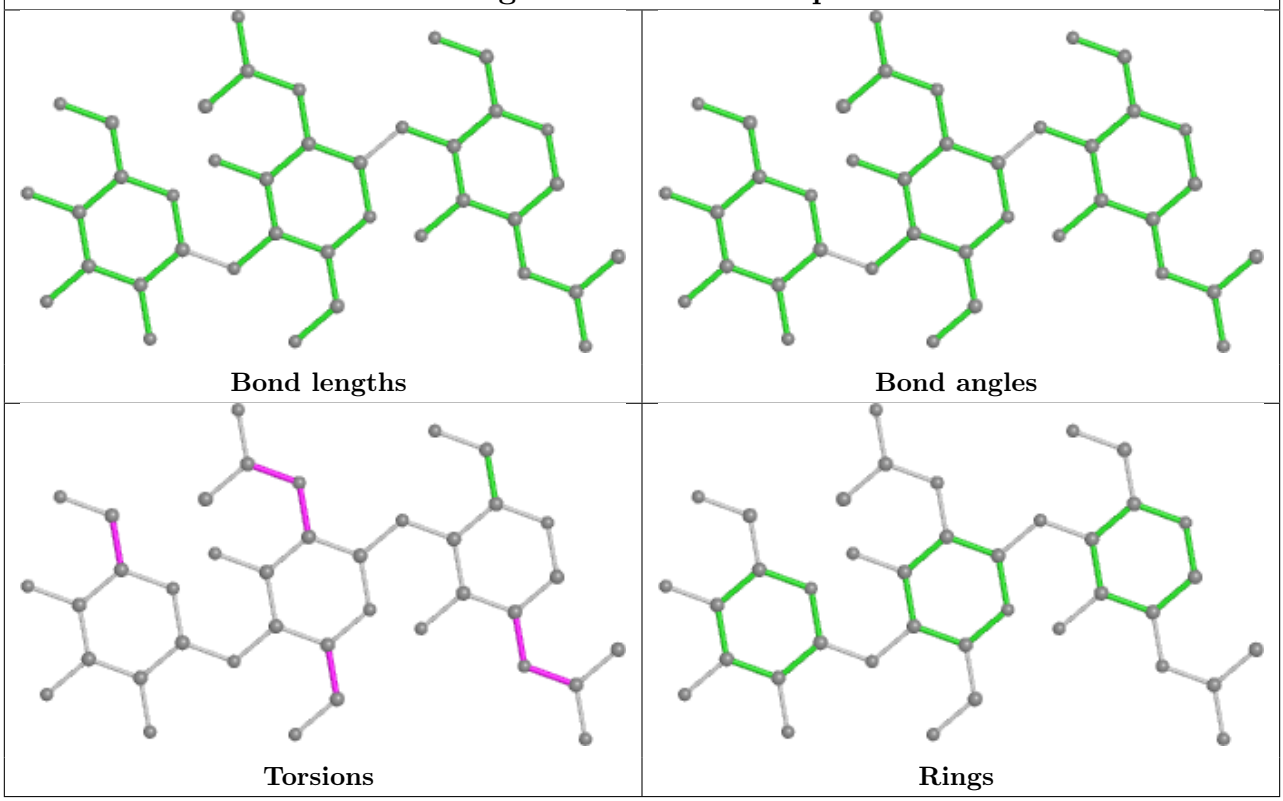


Rings

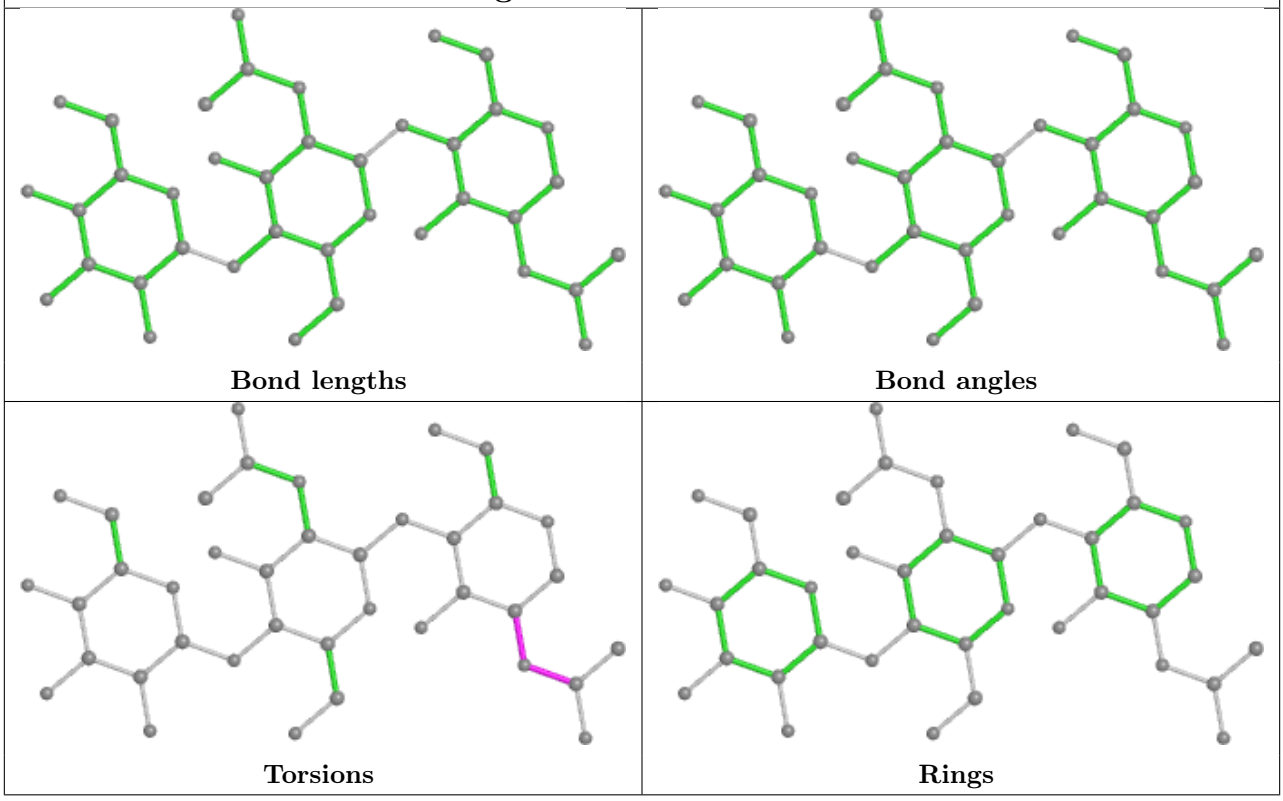
Oligosaccharide Chain k



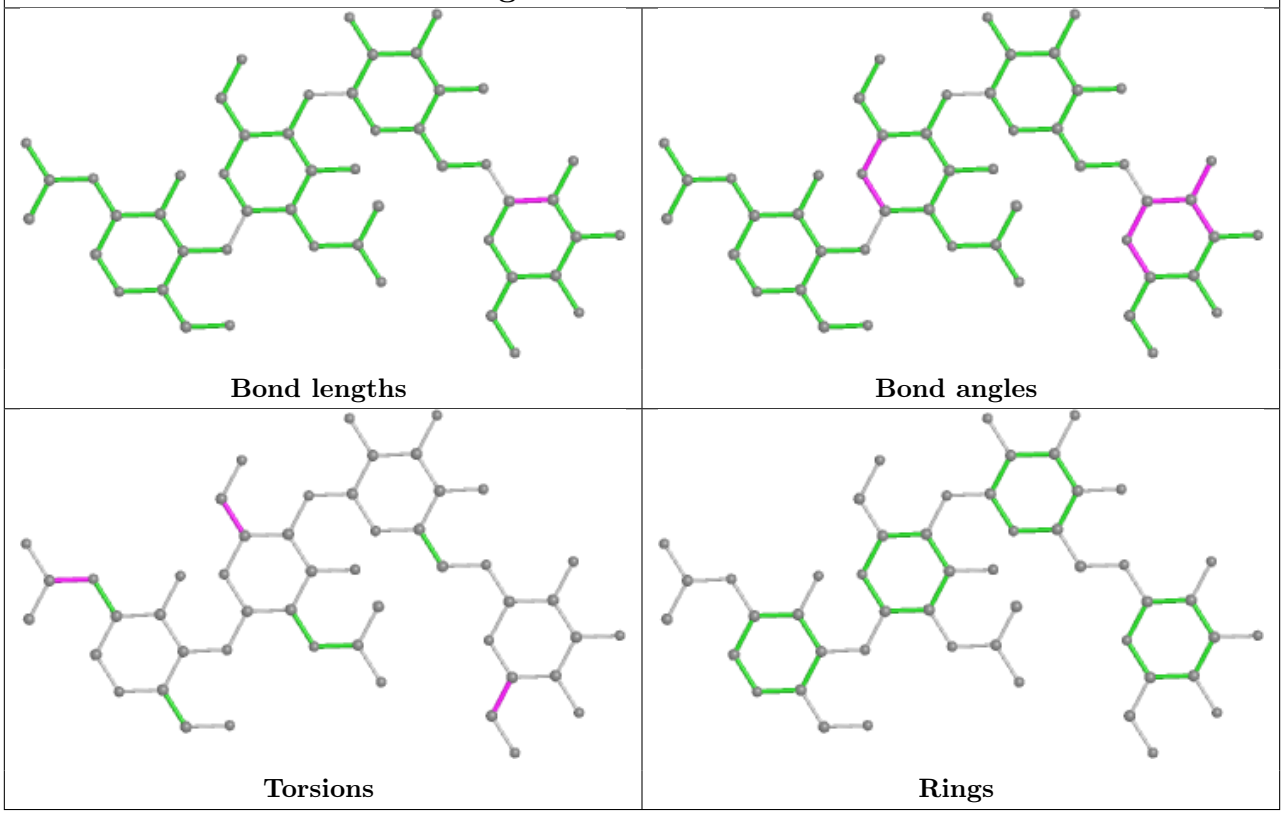
Oligosaccharide Chain p



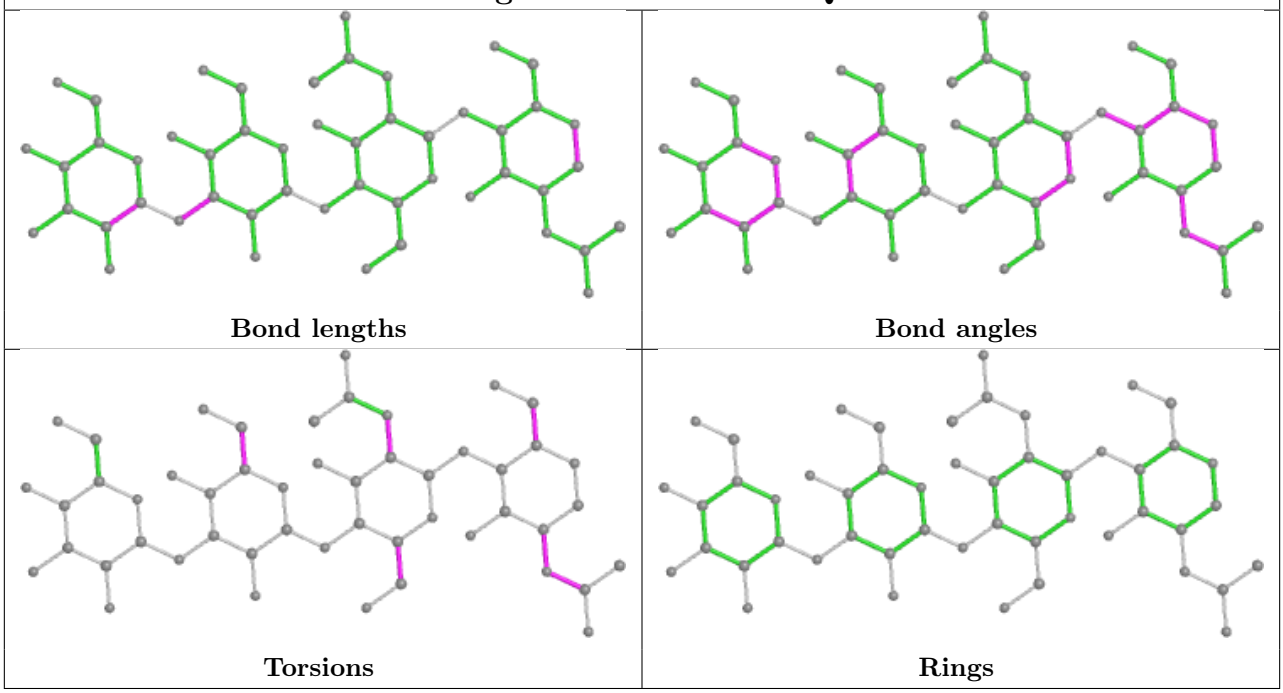
Oligosaccharide Chain V



Oligosaccharide Chain h



Oligosaccharide Chain Q



5.6 Ligand geometry (i)

23 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	$\#\|Z\| > 2$
7	NAG	B	1202	1	14,14,15	0.39	0	17,19,21	0.61	0
7	NAG	A	1206	1	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	B	1203	1	14,14,15	0.59	1 (7%)	17,19,21	0.54	0
7	NAG	C	1201	1	14,14,15	0.22	0	17,19,21	0.55	0
7	NAG	B	1201	1	14,14,15	0.27	0	17,19,21	0.62	0
7	NAG	C	1205	1	14,14,15	0.30	0	17,19,21	0.58	0
7	NAG	B	1205	1	14,14,15	1.65	1 (7%)	17,19,21	0.97	1 (5%)
7	NAG	C	1206	1	14,14,15	0.49	0	17,19,21	1.17	2 (11%)
7	NAG	B	1204	1	14,14,15	0.47	0	17,19,21	1.23	1 (5%)
7	NAG	A	1207	1	14,14,15	0.92	1 (7%)	17,19,21	1.41	2 (11%)
7	NAG	B	1208	1	14,14,15	0.80	1 (7%)	17,19,21	0.52	0
7	NAG	B	1206	1	14,14,15	0.21	0	17,19,21	0.70	1 (5%)
7	NAG	C	1204	-	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
7	NAG	B	1209	1	14,14,15	0.27	0	17,19,21	0.69	0
7	NAG	C	1207	1	14,14,15	0.26	0	17,19,21	0.72	0
7	NAG	A	1203	1	14,14,15	0.29	0	17,19,21	0.61	0
7	NAG	C	1203	1	14,14,15	0.38	0	17,19,21	0.45	0
7	NAG	A	1202	1	14,14,15	0.20	0	17,19,21	0.55	0
7	NAG	A	1201	1	14,14,15	0.59	0	17,19,21	0.80	0
7	NAG	B	1207	1	14,14,15	0.29	0	17,19,21	0.40	0
7	NAG	C	1202	1	14,14,15	0.69	1 (7%)	17,19,21	1.25	2 (11%)
7	NAG	A	1205	1	14,14,15	0.40	0	17,19,21	1.41	2 (11%)
7	NAG	A	1204	1	14,14,15	0.23	0	17,19,21	0.64	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
7	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1206	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1203	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1201	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1205	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1205	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1206	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1204	1	-	5/6/23/26	0/1/1/1
7	NAG	A	1207	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1204	-	-	1/6/23/26	0/1/1/1
7	NAG	B	1209	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1203	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1201	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1207	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1202	1	-	5/6/23/26	0/1/1/1
7	NAG	A	1205	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1204	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1205	NAG	O5-C1	-5.83	1.34	1.43
7	A	1207	NAG	C1-C2	3.03	1.56	1.52
7	B	1208	NAG	O5-C1	-2.58	1.39	1.43
7	C	1202	NAG	O5-C1	-2.36	1.40	1.43
7	B	1203	NAG	C1-C2	2.01	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1205	NAG	C2-N2-C7	4.43	129.22	122.90
7	B	1204	NAG	C2-N2-C7	4.26	128.97	122.90
7	C	1202	NAG	C2-N2-C7	4.11	128.75	122.90
7	A	1207	NAG	C2-N2-C7	3.85	128.38	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1206	NAG	C2-N2-C7	3.51	127.90	122.90
7	A	1207	NAG	C1-O5-C5	3.31	116.67	112.19
7	B	1205	NAG	C3-C4-C5	2.84	115.30	110.24
7	A	1205	NAG	C1-C2-N2	2.69	115.08	110.49
7	C	1204	NAG	C1-O5-C5	2.35	115.38	112.19
7	B	1206	NAG	C1-O5-C5	2.27	115.27	112.19
7	C	1206	NAG	C1-C2-N2	2.09	114.05	110.49
7	C	1202	NAG	C1-C2-N2	2.06	114.01	110.49

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1209	NAG	C3-C2-N2-C7
7	B	1208	NAG	O5-C5-C6-O6
7	A	1202	NAG	C4-C5-C6-O6
7	B	1204	NAG	O5-C5-C6-O6
7	B	1206	NAG	C4-C5-C6-O6
7	B	1206	NAG	O5-C5-C6-O6
7	B	1202	NAG	O5-C5-C6-O6
7	B	1208	NAG	C4-C5-C6-O6
7	B	1203	NAG	O5-C5-C6-O6
7	A	1202	NAG	O5-C5-C6-O6
7	C	1203	NAG	O5-C5-C6-O6
7	A	1201	NAG	C1-C2-N2-C7
7	C	1203	NAG	C4-C5-C6-O6
7	A	1205	NAG	C8-C7-N2-C2
7	A	1205	NAG	O7-C7-N2-C2
7	A	1207	NAG	C8-C7-N2-C2
7	A	1207	NAG	O7-C7-N2-C2
7	B	1204	NAG	C8-C7-N2-C2
7	B	1204	NAG	O7-C7-N2-C2
7	C	1202	NAG	C8-C7-N2-C2
7	C	1202	NAG	O7-C7-N2-C2
7	C	1203	NAG	C8-C7-N2-C2
7	C	1203	NAG	O7-C7-N2-C2
7	C	1205	NAG	C8-C7-N2-C2
7	C	1205	NAG	O7-C7-N2-C2
7	C	1206	NAG	C8-C7-N2-C2
7	C	1206	NAG	O7-C7-N2-C2
7	B	1207	NAG	O5-C5-C6-O6
7	B	1205	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	1203	NAG	C4-C5-C6-O6
7	B	1205	NAG	C4-C5-C6-O6
7	B	1204	NAG	C4-C5-C6-O6
7	B	1203	NAG	C1-C2-N2-C7
7	A	1204	NAG	O5-C5-C6-O6
7	A	1201	NAG	O5-C5-C6-O6
7	B	1205	NAG	C1-C2-N2-C7
7	C	1205	NAG	O5-C5-C6-O6
7	B	1201	NAG	O5-C5-C6-O6
7	C	1202	NAG	C4-C5-C6-O6
7	C	1201	NAG	C4-C5-C6-O6
7	C	1202	NAG	O5-C5-C6-O6
7	A	1207	NAG	C4-C5-C6-O6
7	A	1204	NAG	C4-C5-C6-O6
7	A	1206	NAG	C1-C2-N2-C7
7	A	1201	NAG	C3-C2-N2-C7
7	A	1205	NAG	C3-C2-N2-C7
7	B	1201	NAG	C3-C2-N2-C7
7	B	1205	NAG	C3-C2-N2-C7
7	C	1202	NAG	C3-C2-N2-C7
7	C	1204	NAG	C3-C2-N2-C7
7	C	1205	NAG	C3-C2-N2-C7
7	C	1201	NAG	O5-C5-C6-O6
7	B	1202	NAG	C4-C5-C6-O6
7	B	1207	NAG	C4-C5-C6-O6
7	B	1201	NAG	C4-C5-C6-O6
7	A	1207	NAG	C3-C2-N2-C7
7	B	1203	NAG	C3-C2-N2-C7
7	B	1204	NAG	C3-C2-N2-C7
7	C	1206	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

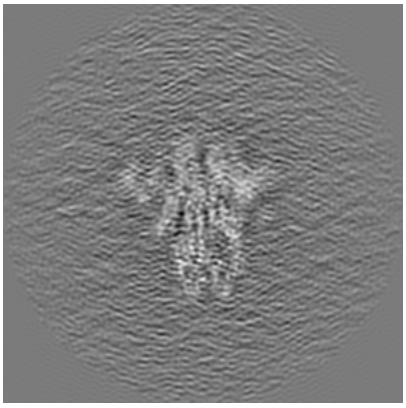
6 Map visualisation (i)

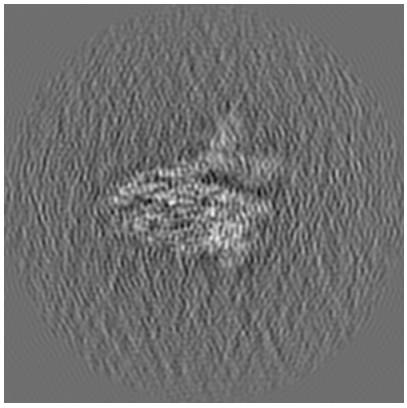
This section contains visualisations of the EMDB entry EMD-30419. These allow visual inspection of the internal detail of the map and identification of artifacts.

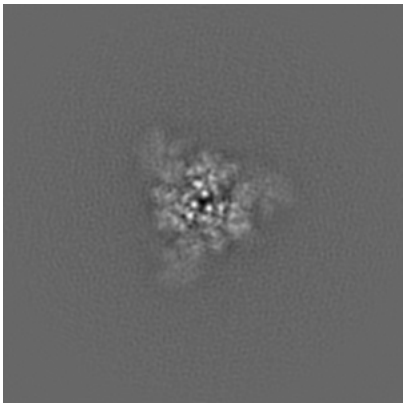
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

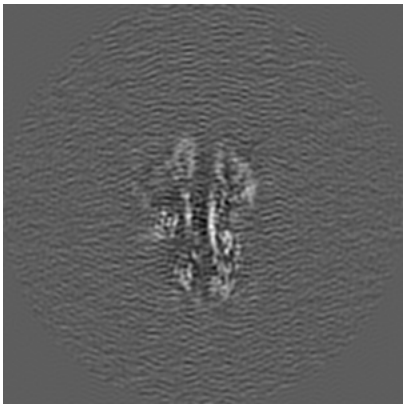

Y

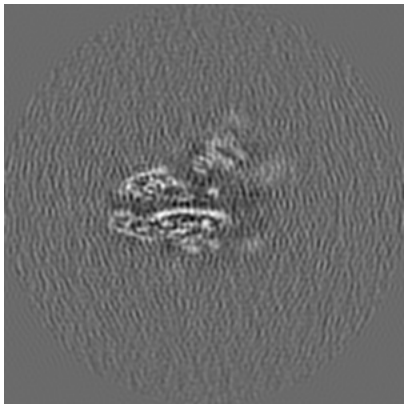

Z

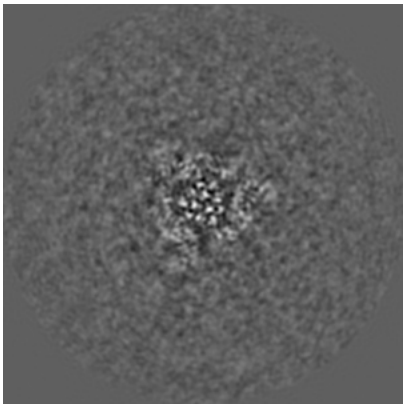
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 216

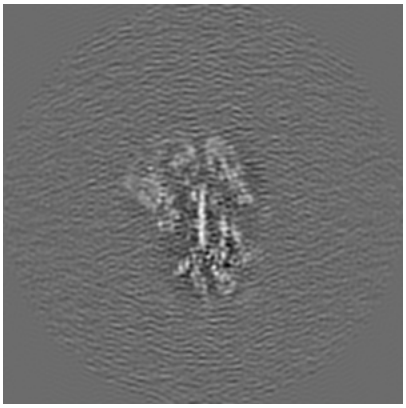

Y Index: 216


Z Index: 216

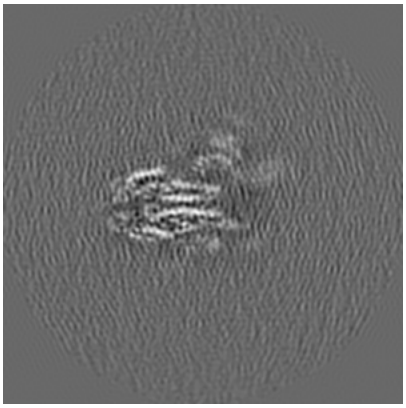
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

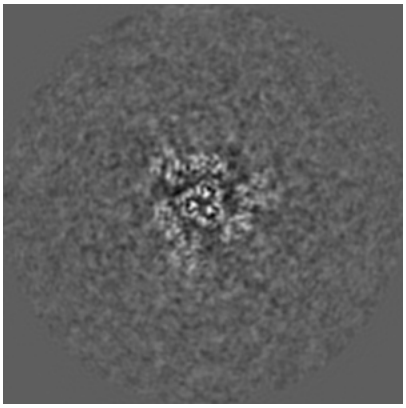
6.3.1 Primary map



X Index: 207



Y Index: 213



Z Index: 224

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 0.00738. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

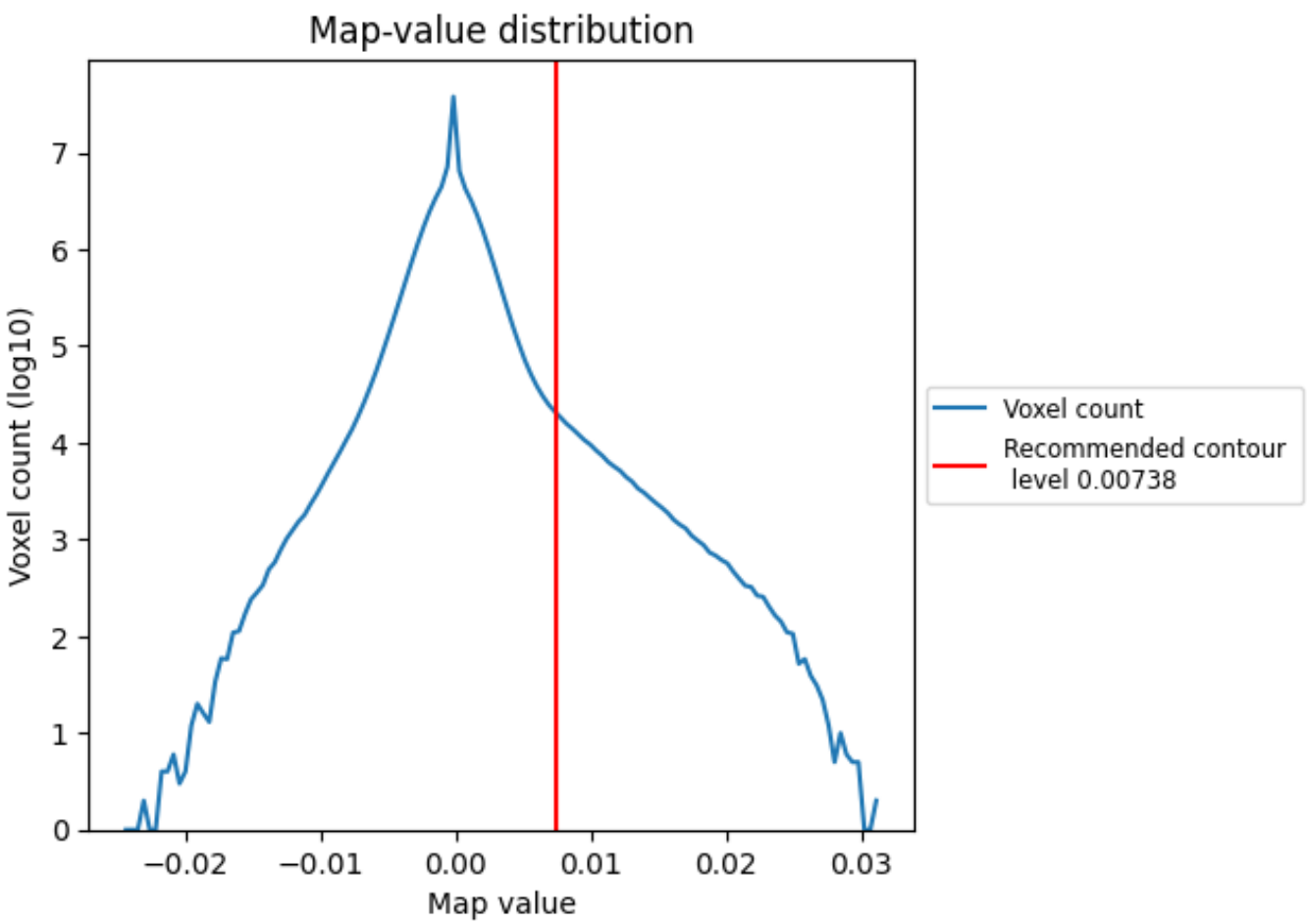
6.5 Mask visualisation (i)

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

7 Map analysis (i)

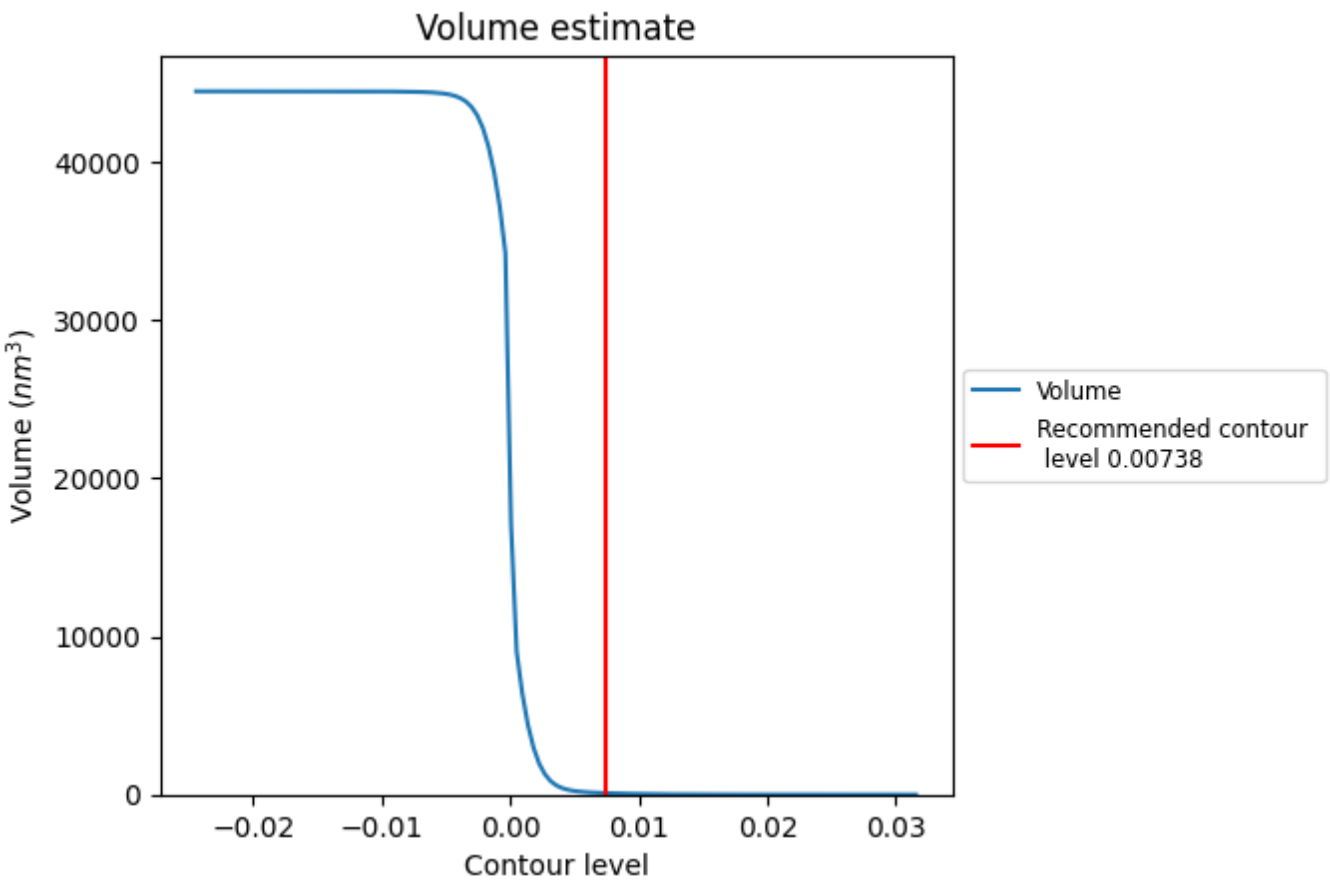
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

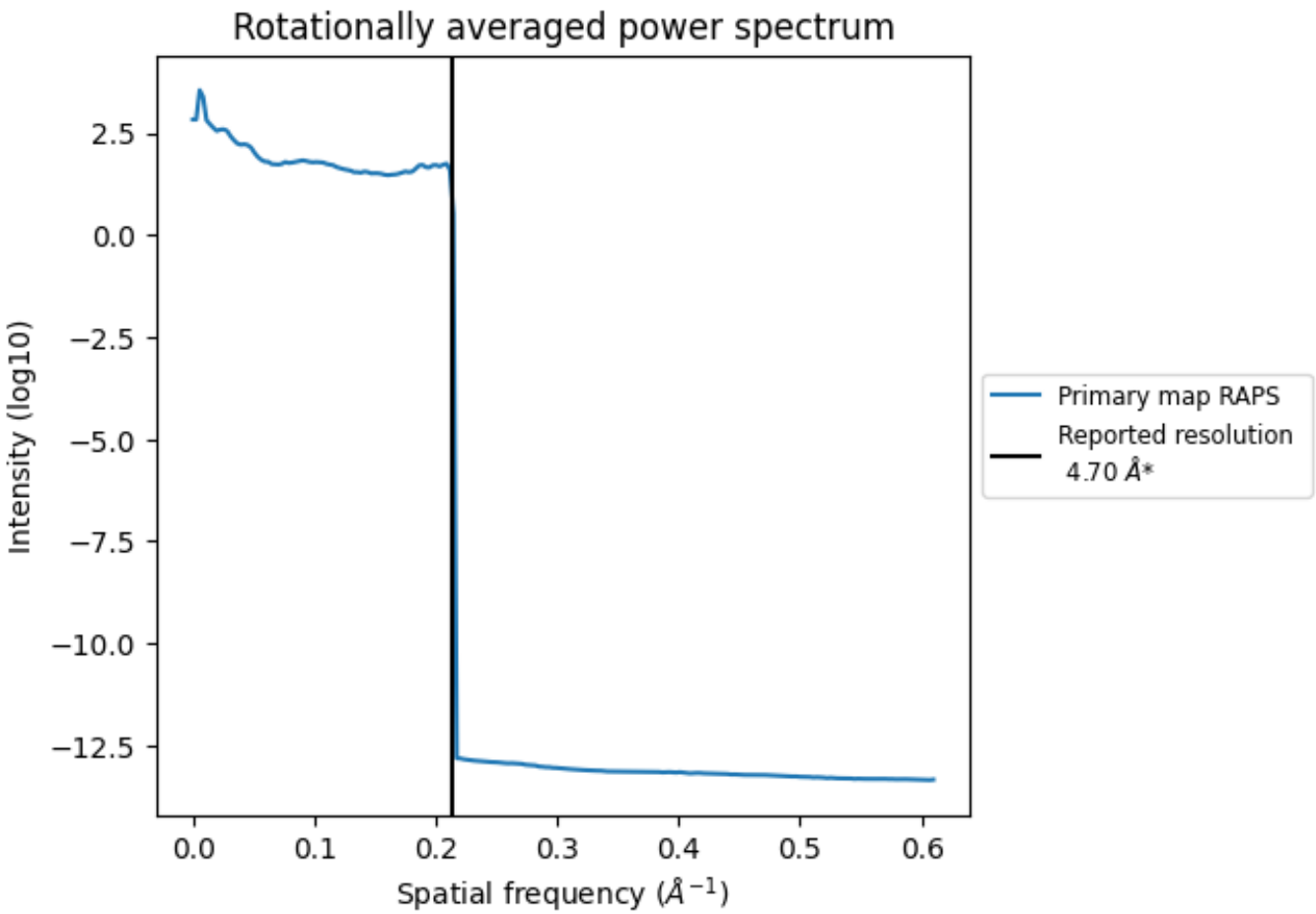
7.2 Volume estimate (i)



The volume at the recommended contour level is 92 nm^3; this corresponds to an approximate mass of 84 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 0.213 Å^{-1}

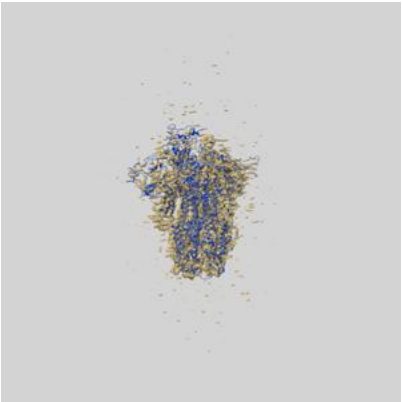
8 Fourier-Shell correlation (i)

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

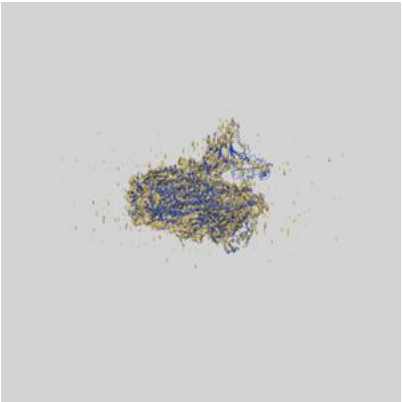
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30419 and PDB model 7CN9. Per-residue inclusion information can be found in section 3 on page 9.

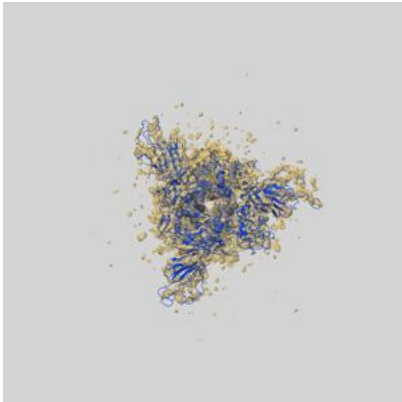
9.1 Map-model overlay (i)



X



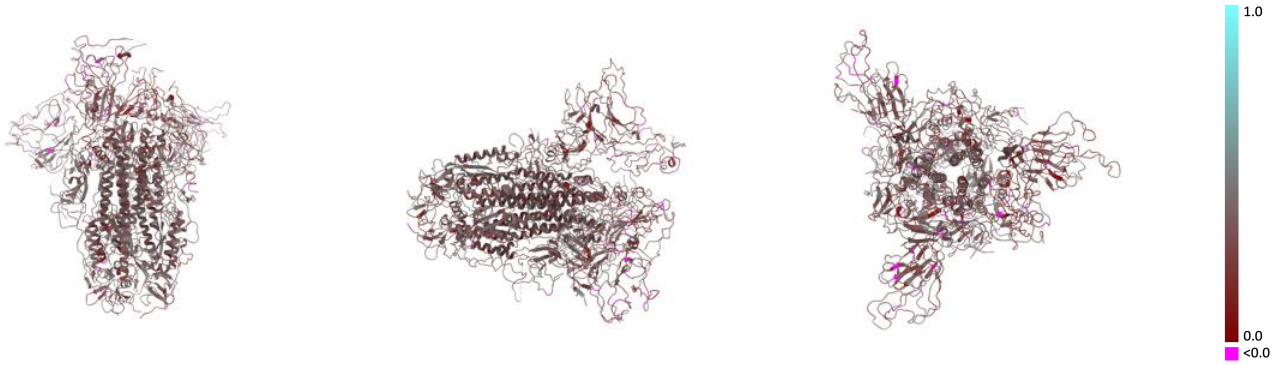
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00738 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.

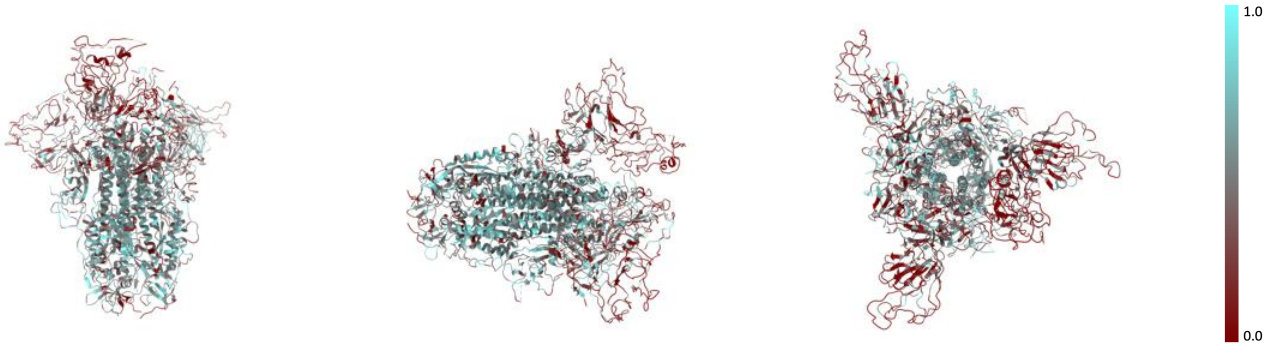
9.2 Q-score mapped to coordinate model (i)



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.

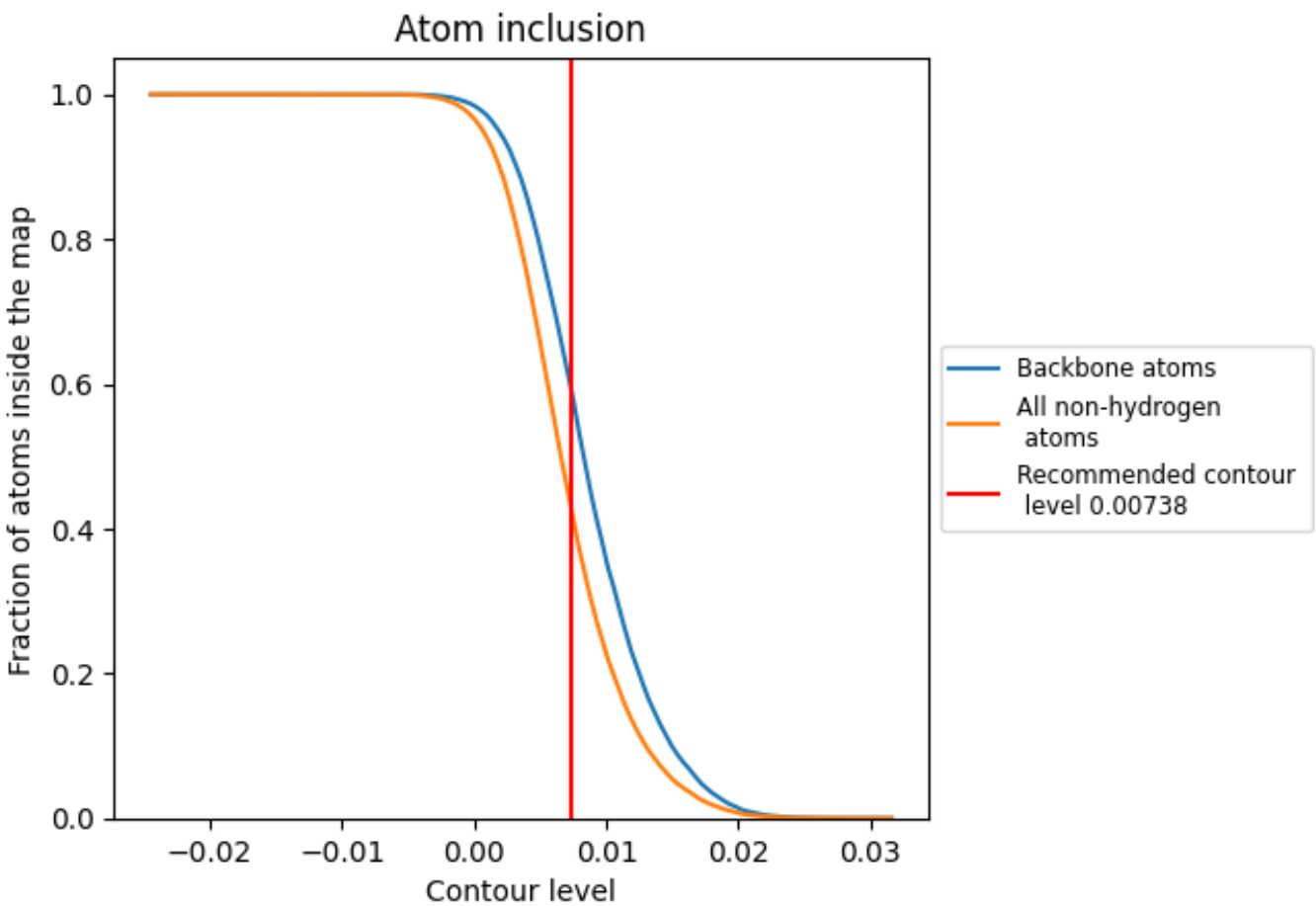
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00738).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00738) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4247	0.3410
A	0.3973	0.3420
B	0.4409	0.3360
C	0.4447	0.3410
E	0.1071	0.4070
H	0.3571	0.3700
N	0.0714	0.4400
Q	0.2200	0.3940
V	0.2308	0.2700
W	0.4643	0.4540
X	0.2857	0.4050
Z	0.0000	0.4640
d	0.3214	0.4190
f	0.5357	0.4710
h	0.0800	0.4670
k	0.3947	0.4780
p	0.4103	0.3900