wwPDB EM Validation Summary Report

Nov 29, 2022 – 03:29 AM EST

PDB ID	:	7USA
EMDB ID	:	EMD-26730
Title	:	Structure of the human coronavirus CCoV-HuPn-2018 spike glycoprotein with domain 0 in the swung out conformation
Authors	:	Tortorici, M.A.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2022-04-23
Resolution	:	2.80 Å(reported)

This is a wwPDB EM Validation Summary 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:

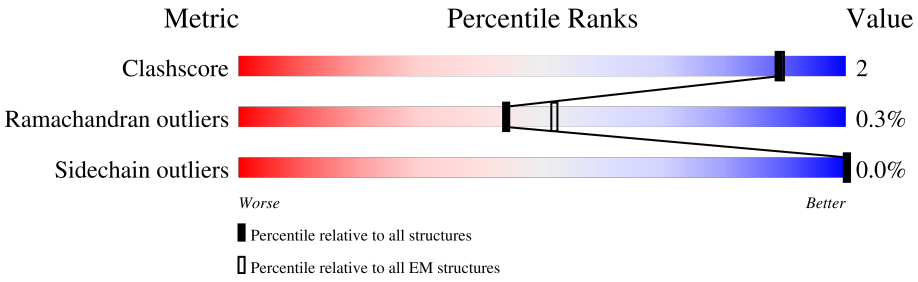
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	1469	8% 70% · 28%
1	B	1469	8% 69% · 28%
1	C	1469	9% 70% · 28%
2	D	2	50% 100%
2	E	2	50% 100%
2	F	2	100%
2	G	2	100%
2	H	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
2	I	2	50% 100%
2	K	2	50% 100%
2	M	2	100% 100%
2	N	2	50% 100%
2	O	2	100%
2	P	2	100%
2	Q	2	50% 50% 50%
2	R	2	50% 100%
2	T	2	50% 100%
2	V	2	50% 100%
2	W	2	50% 100%
2	X	2	100%
2	Y	2	100%
2	Z	2	50% 50% 50%
2	a	2	50% 100%
2	c	2	50% 100%
3	J	3	33% 100%
3	L	3	33% 100%
3	S	3	33% 100%
3	U	3	33% 100%
3	b	3	33% 100%
3	d	3	33% 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	A	1508	X	-	-	-
4	NAG	B	1508	X	-	-	-
4	NAG	C	1508	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			7694	4926	1297	1429	42		
1	B	1058	Total	C	N	O	S	0	0
			7678	4903	1296	1437	42		
1	C	1062	Total	C	N	O	S	0	0
			7693	4916	1296	1439	42		

There are 297 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP A0A8E6CMP0
A	-14	GLY	-	expression tag	UNP A0A8E6CMP0
A	-13	ILE	-	expression tag	UNP A0A8E6CMP0
A	-12	LEU	-	expression tag	UNP A0A8E6CMP0
A	-11	PRO	-	expression tag	UNP A0A8E6CMP0
A	-10	SER	-	expression tag	UNP A0A8E6CMP0
A	-9	PRO	-	expression tag	UNP A0A8E6CMP0
A	-8	GLY	-	expression tag	UNP A0A8E6CMP0
A	-7	MET	-	expression tag	UNP A0A8E6CMP0
A	-6	PRO	-	expression tag	UNP A0A8E6CMP0
A	-5	ALA	-	expression tag	UNP A0A8E6CMP0
A	-4	LEU	-	expression tag	UNP A0A8E6CMP0
A	-3	LEU	-	expression tag	UNP A0A8E6CMP0
A	-2	SER	-	expression tag	UNP A0A8E6CMP0
A	-1	LEU	-	expression tag	UNP A0A8E6CMP0
A	0	VAL	-	expression tag	UNP A0A8E6CMP0
A	1	SER	-	expression tag	UNP A0A8E6CMP0
A	2	LEU	-	expression tag	UNP A0A8E6CMP0
A	3	LEU	-	expression tag	UNP A0A8E6CMP0
A	4	SER	-	expression tag	UNP A0A8E6CMP0
A	5	VAL	-	expression tag	UNP A0A8E6CMP0
A	6	LEU	-	expression tag	UNP A0A8E6CMP0
A	7	LEU	-	expression tag	UNP A0A8E6CMP0
A	8	MET	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP A0A8E6CMP0
A	10	CYS	-	expression tag	UNP A0A8E6CMP0
A	11	VAL	-	expression tag	UNP A0A8E6CMP0
A	12	ALA	-	expression tag	UNP A0A8E6CMP0
A	13	GLU	-	expression tag	UNP A0A8E6CMP0
A	14	THR	-	expression tag	UNP A0A8E6CMP0
A	15	GLY	-	expression tag	UNP A0A8E6CMP0
A	16	THR	-	expression tag	UNP A0A8E6CMP0
A	1140	PRO	GLU	conflict	UNP A0A8E6CMP0
A	1141	PRO	LEU	conflict	UNP A0A8E6CMP0
A	1388	SER	TRP	conflict	UNP A0A8E6CMP0
A	1389	GLY	PRO	conflict	UNP A0A8E6CMP0
A	1390	GLY	TRP	conflict	UNP A0A8E6CMP0
A	1392	ILE	VAL	conflict	UNP A0A8E6CMP0
A	1393	PRO	-	expression tag	UNP A0A8E6CMP0
A	1394	GLU	-	expression tag	UNP A0A8E6CMP0
A	1395	ALA	-	expression tag	UNP A0A8E6CMP0
A	1396	PRO	-	expression tag	UNP A0A8E6CMP0
A	1397	ARG	-	expression tag	UNP A0A8E6CMP0
A	1398	ASP	-	expression tag	UNP A0A8E6CMP0
A	1399	GLY	-	expression tag	UNP A0A8E6CMP0
A	1400	GLN	-	expression tag	UNP A0A8E6CMP0
A	1401	ALA	-	expression tag	UNP A0A8E6CMP0
A	1402	TYR	-	expression tag	UNP A0A8E6CMP0
A	1403	VAL	-	expression tag	UNP A0A8E6CMP0
A	1404	ARG	-	expression tag	UNP A0A8E6CMP0
A	1405	LYS	-	expression tag	UNP A0A8E6CMP0
A	1406	ASP	-	expression tag	UNP A0A8E6CMP0
A	1407	GLY	-	expression tag	UNP A0A8E6CMP0
A	1408	GLU	-	expression tag	UNP A0A8E6CMP0
A	1409	TRP	-	expression tag	UNP A0A8E6CMP0
A	1410	VAL	-	expression tag	UNP A0A8E6CMP0
A	1411	LEU	-	expression tag	UNP A0A8E6CMP0
A	1412	LEU	-	expression tag	UNP A0A8E6CMP0
A	1413	SER	-	expression tag	UNP A0A8E6CMP0
A	1414	THR	-	expression tag	UNP A0A8E6CMP0
A	1415	PHE	-	expression tag	UNP A0A8E6CMP0
A	1416	LEU	-	expression tag	UNP A0A8E6CMP0
A	1417	VAL	-	expression tag	UNP A0A8E6CMP0
A	1418	PRO	-	expression tag	UNP A0A8E6CMP0
A	1419	ARG	-	expression tag	UNP A0A8E6CMP0
A	1420	GLY	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1421	SER	-	expression tag	UNP A0A8E6CMP0
A	1422	GLY	-	expression tag	UNP A0A8E6CMP0
A	1423	GLY	-	expression tag	UNP A0A8E6CMP0
A	1424	SER	-	expression tag	UNP A0A8E6CMP0
A	1425	GLY	-	expression tag	UNP A0A8E6CMP0
A	1426	GLY	-	expression tag	UNP A0A8E6CMP0
A	1427	SER	-	expression tag	UNP A0A8E6CMP0
A	1428	GLY	-	expression tag	UNP A0A8E6CMP0
A	1429	LEU	-	expression tag	UNP A0A8E6CMP0
A	1430	ASN	-	expression tag	UNP A0A8E6CMP0
A	1431	ASP	-	expression tag	UNP A0A8E6CMP0
A	1432	ILE	-	expression tag	UNP A0A8E6CMP0
A	1433	PHE	-	expression tag	UNP A0A8E6CMP0
A	1434	GLU	-	expression tag	UNP A0A8E6CMP0
A	1435	ALA	-	expression tag	UNP A0A8E6CMP0
A	1436	GLN	-	expression tag	UNP A0A8E6CMP0
A	1437	LYS	-	expression tag	UNP A0A8E6CMP0
A	1438	ILE	-	expression tag	UNP A0A8E6CMP0
A	1439	GLU	-	expression tag	UNP A0A8E6CMP0
A	1440	TRP	-	expression tag	UNP A0A8E6CMP0
A	1441	HIS	-	expression tag	UNP A0A8E6CMP0
A	1442	GLU	-	expression tag	UNP A0A8E6CMP0
A	1443	GLY	-	expression tag	UNP A0A8E6CMP0
A	1444	GLY	-	expression tag	UNP A0A8E6CMP0
A	1445	SER	-	expression tag	UNP A0A8E6CMP0
A	1446	HIS	-	expression tag	UNP A0A8E6CMP0
A	1447	HIS	-	expression tag	UNP A0A8E6CMP0
A	1448	HIS	-	expression tag	UNP A0A8E6CMP0
A	1449	HIS	-	expression tag	UNP A0A8E6CMP0
A	1450	HIS	-	expression tag	UNP A0A8E6CMP0
A	1451	HIS	-	expression tag	UNP A0A8E6CMP0
A	1452	HIS	-	expression tag	UNP A0A8E6CMP0
A	1453	HIS	-	expression tag	UNP A0A8E6CMP0
B	-15	MET	-	initiating methionine	UNP A0A8E6CMP0
B	-14	GLY	-	expression tag	UNP A0A8E6CMP0
B	-13	ILE	-	expression tag	UNP A0A8E6CMP0
B	-12	LEU	-	expression tag	UNP A0A8E6CMP0
B	-11	PRO	-	expression tag	UNP A0A8E6CMP0
B	-10	SER	-	expression tag	UNP A0A8E6CMP0
B	-9	PRO	-	expression tag	UNP A0A8E6CMP0
B	-8	GLY	-	expression tag	UNP A0A8E6CMP0
B	-7	MET	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PRO	-	expression tag	UNP A0A8E6CMP0
B	-5	ALA	-	expression tag	UNP A0A8E6CMP0
B	-4	LEU	-	expression tag	UNP A0A8E6CMP0
B	-3	LEU	-	expression tag	UNP A0A8E6CMP0
B	-2	SER	-	expression tag	UNP A0A8E6CMP0
B	-1	LEU	-	expression tag	UNP A0A8E6CMP0
B	0	VAL	-	expression tag	UNP A0A8E6CMP0
B	1	SER	-	expression tag	UNP A0A8E6CMP0
B	2	LEU	-	expression tag	UNP A0A8E6CMP0
B	3	LEU	-	expression tag	UNP A0A8E6CMP0
B	4	SER	-	expression tag	UNP A0A8E6CMP0
B	5	VAL	-	expression tag	UNP A0A8E6CMP0
B	6	LEU	-	expression tag	UNP A0A8E6CMP0
B	7	LEU	-	expression tag	UNP A0A8E6CMP0
B	8	MET	-	expression tag	UNP A0A8E6CMP0
B	9	GLY	-	expression tag	UNP A0A8E6CMP0
B	10	CYS	-	expression tag	UNP A0A8E6CMP0
B	11	VAL	-	expression tag	UNP A0A8E6CMP0
B	12	ALA	-	expression tag	UNP A0A8E6CMP0
B	13	GLU	-	expression tag	UNP A0A8E6CMP0
B	14	THR	-	expression tag	UNP A0A8E6CMP0
B	15	GLY	-	expression tag	UNP A0A8E6CMP0
B	16	THR	-	expression tag	UNP A0A8E6CMP0
B	1140	PRO	GLU	conflict	UNP A0A8E6CMP0
B	1141	PRO	LEU	conflict	UNP A0A8E6CMP0
B	1388	SER	TRP	conflict	UNP A0A8E6CMP0
B	1389	GLY	PRO	conflict	UNP A0A8E6CMP0
B	1390	GLY	TRP	conflict	UNP A0A8E6CMP0
B	1392	ILE	VAL	conflict	UNP A0A8E6CMP0
B	1393	PRO	-	expression tag	UNP A0A8E6CMP0
B	1394	GLU	-	expression tag	UNP A0A8E6CMP0
B	1395	ALA	-	expression tag	UNP A0A8E6CMP0
B	1396	PRO	-	expression tag	UNP A0A8E6CMP0
B	1397	ARG	-	expression tag	UNP A0A8E6CMP0
B	1398	ASP	-	expression tag	UNP A0A8E6CMP0
B	1399	GLY	-	expression tag	UNP A0A8E6CMP0
B	1400	GLN	-	expression tag	UNP A0A8E6CMP0
B	1401	ALA	-	expression tag	UNP A0A8E6CMP0
B	1402	TYR	-	expression tag	UNP A0A8E6CMP0
B	1403	VAL	-	expression tag	UNP A0A8E6CMP0
B	1404	ARG	-	expression tag	UNP A0A8E6CMP0
B	1405	LYS	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1406	ASP	-	expression tag	UNP A0A8E6CMP0
B	1407	GLY	-	expression tag	UNP A0A8E6CMP0
B	1408	GLU	-	expression tag	UNP A0A8E6CMP0
B	1409	TRP	-	expression tag	UNP A0A8E6CMP0
B	1410	VAL	-	expression tag	UNP A0A8E6CMP0
B	1411	LEU	-	expression tag	UNP A0A8E6CMP0
B	1412	LEU	-	expression tag	UNP A0A8E6CMP0
B	1413	SER	-	expression tag	UNP A0A8E6CMP0
B	1414	THR	-	expression tag	UNP A0A8E6CMP0
B	1415	PHE	-	expression tag	UNP A0A8E6CMP0
B	1416	LEU	-	expression tag	UNP A0A8E6CMP0
B	1417	VAL	-	expression tag	UNP A0A8E6CMP0
B	1418	PRO	-	expression tag	UNP A0A8E6CMP0
B	1419	ARG	-	expression tag	UNP A0A8E6CMP0
B	1420	GLY	-	expression tag	UNP A0A8E6CMP0
B	1421	SER	-	expression tag	UNP A0A8E6CMP0
B	1422	GLY	-	expression tag	UNP A0A8E6CMP0
B	1423	GLY	-	expression tag	UNP A0A8E6CMP0
B	1424	SER	-	expression tag	UNP A0A8E6CMP0
B	1425	GLY	-	expression tag	UNP A0A8E6CMP0
B	1426	GLY	-	expression tag	UNP A0A8E6CMP0
B	1427	SER	-	expression tag	UNP A0A8E6CMP0
B	1428	GLY	-	expression tag	UNP A0A8E6CMP0
B	1429	LEU	-	expression tag	UNP A0A8E6CMP0
B	1430	ASN	-	expression tag	UNP A0A8E6CMP0
B	1431	ASP	-	expression tag	UNP A0A8E6CMP0
B	1432	ILE	-	expression tag	UNP A0A8E6CMP0
B	1433	PHE	-	expression tag	UNP A0A8E6CMP0
B	1434	GLU	-	expression tag	UNP A0A8E6CMP0
B	1435	ALA	-	expression tag	UNP A0A8E6CMP0
B	1436	GLN	-	expression tag	UNP A0A8E6CMP0
B	1437	LYS	-	expression tag	UNP A0A8E6CMP0
B	1438	ILE	-	expression tag	UNP A0A8E6CMP0
B	1439	GLU	-	expression tag	UNP A0A8E6CMP0
B	1440	TRP	-	expression tag	UNP A0A8E6CMP0
B	1441	HIS	-	expression tag	UNP A0A8E6CMP0
B	1442	GLU	-	expression tag	UNP A0A8E6CMP0
B	1443	GLY	-	expression tag	UNP A0A8E6CMP0
B	1444	GLY	-	expression tag	UNP A0A8E6CMP0
B	1445	SER	-	expression tag	UNP A0A8E6CMP0
B	1446	HIS	-	expression tag	UNP A0A8E6CMP0
B	1447	HIS	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1448	HIS	-	expression tag	UNP A0A8E6CMP0
B	1449	HIS	-	expression tag	UNP A0A8E6CMP0
B	1450	HIS	-	expression tag	UNP A0A8E6CMP0
B	1451	HIS	-	expression tag	UNP A0A8E6CMP0
B	1452	HIS	-	expression tag	UNP A0A8E6CMP0
B	1453	HIS	-	expression tag	UNP A0A8E6CMP0
C	-15	MET	-	initiating methionine	UNP A0A8E6CMP0
C	-14	GLY	-	expression tag	UNP A0A8E6CMP0
C	-13	ILE	-	expression tag	UNP A0A8E6CMP0
C	-12	LEU	-	expression tag	UNP A0A8E6CMP0
C	-11	PRO	-	expression tag	UNP A0A8E6CMP0
C	-10	SER	-	expression tag	UNP A0A8E6CMP0
C	-9	PRO	-	expression tag	UNP A0A8E6CMP0
C	-8	GLY	-	expression tag	UNP A0A8E6CMP0
C	-7	MET	-	expression tag	UNP A0A8E6CMP0
C	-6	PRO	-	expression tag	UNP A0A8E6CMP0
C	-5	ALA	-	expression tag	UNP A0A8E6CMP0
C	-4	LEU	-	expression tag	UNP A0A8E6CMP0
C	-3	LEU	-	expression tag	UNP A0A8E6CMP0
C	-2	SER	-	expression tag	UNP A0A8E6CMP0
C	-1	LEU	-	expression tag	UNP A0A8E6CMP0
C	0	VAL	-	expression tag	UNP A0A8E6CMP0
C	1	SER	-	expression tag	UNP A0A8E6CMP0
C	2	LEU	-	expression tag	UNP A0A8E6CMP0
C	3	LEU	-	expression tag	UNP A0A8E6CMP0
C	4	SER	-	expression tag	UNP A0A8E6CMP0
C	5	VAL	-	expression tag	UNP A0A8E6CMP0
C	6	LEU	-	expression tag	UNP A0A8E6CMP0
C	7	LEU	-	expression tag	UNP A0A8E6CMP0
C	8	MET	-	expression tag	UNP A0A8E6CMP0
C	9	GLY	-	expression tag	UNP A0A8E6CMP0
C	10	CYS	-	expression tag	UNP A0A8E6CMP0
C	11	VAL	-	expression tag	UNP A0A8E6CMP0
C	12	ALA	-	expression tag	UNP A0A8E6CMP0
C	13	GLU	-	expression tag	UNP A0A8E6CMP0
C	14	THR	-	expression tag	UNP A0A8E6CMP0
C	15	GLY	-	expression tag	UNP A0A8E6CMP0
C	16	THR	-	expression tag	UNP A0A8E6CMP0
C	1140	PRO	GLU	conflict	UNP A0A8E6CMP0
C	1141	PRO	LEU	conflict	UNP A0A8E6CMP0
C	1388	SER	TRP	conflict	UNP A0A8E6CMP0
C	1389	GLY	PRO	conflict	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1390	GLY	TRP	conflict	UNP A0A8E6CMP0
C	1392	ILE	VAL	conflict	UNP A0A8E6CMP0
C	1393	PRO	-	expression tag	UNP A0A8E6CMP0
C	1394	GLU	-	expression tag	UNP A0A8E6CMP0
C	1395	ALA	-	expression tag	UNP A0A8E6CMP0
C	1396	PRO	-	expression tag	UNP A0A8E6CMP0
C	1397	ARG	-	expression tag	UNP A0A8E6CMP0
C	1398	ASP	-	expression tag	UNP A0A8E6CMP0
C	1399	GLY	-	expression tag	UNP A0A8E6CMP0
C	1400	GLN	-	expression tag	UNP A0A8E6CMP0
C	1401	ALA	-	expression tag	UNP A0A8E6CMP0
C	1402	TYR	-	expression tag	UNP A0A8E6CMP0
C	1403	VAL	-	expression tag	UNP A0A8E6CMP0
C	1404	ARG	-	expression tag	UNP A0A8E6CMP0
C	1405	LYS	-	expression tag	UNP A0A8E6CMP0
C	1406	ASP	-	expression tag	UNP A0A8E6CMP0
C	1407	GLY	-	expression tag	UNP A0A8E6CMP0
C	1408	GLU	-	expression tag	UNP A0A8E6CMP0
C	1409	TRP	-	expression tag	UNP A0A8E6CMP0
C	1410	VAL	-	expression tag	UNP A0A8E6CMP0
C	1411	LEU	-	expression tag	UNP A0A8E6CMP0
C	1412	LEU	-	expression tag	UNP A0A8E6CMP0
C	1413	SER	-	expression tag	UNP A0A8E6CMP0
C	1414	THR	-	expression tag	UNP A0A8E6CMP0
C	1415	PHE	-	expression tag	UNP A0A8E6CMP0
C	1416	LEU	-	expression tag	UNP A0A8E6CMP0
C	1417	VAL	-	expression tag	UNP A0A8E6CMP0
C	1418	PRO	-	expression tag	UNP A0A8E6CMP0
C	1419	ARG	-	expression tag	UNP A0A8E6CMP0
C	1420	GLY	-	expression tag	UNP A0A8E6CMP0
C	1421	SER	-	expression tag	UNP A0A8E6CMP0
C	1422	GLY	-	expression tag	UNP A0A8E6CMP0
C	1423	GLY	-	expression tag	UNP A0A8E6CMP0
C	1424	SER	-	expression tag	UNP A0A8E6CMP0
C	1425	GLY	-	expression tag	UNP A0A8E6CMP0
C	1426	GLY	-	expression tag	UNP A0A8E6CMP0
C	1427	SER	-	expression tag	UNP A0A8E6CMP0
C	1428	GLY	-	expression tag	UNP A0A8E6CMP0
C	1429	LEU	-	expression tag	UNP A0A8E6CMP0
C	1430	ASN	-	expression tag	UNP A0A8E6CMP0
C	1431	ASP	-	expression tag	UNP A0A8E6CMP0
C	1432	ILE	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1433	PHE	-	expression tag	UNP A0A8E6CMP0
C	1434	GLU	-	expression tag	UNP A0A8E6CMP0
C	1435	ALA	-	expression tag	UNP A0A8E6CMP0
C	1436	GLN	-	expression tag	UNP A0A8E6CMP0
C	1437	LYS	-	expression tag	UNP A0A8E6CMP0
C	1438	ILE	-	expression tag	UNP A0A8E6CMP0
C	1439	GLU	-	expression tag	UNP A0A8E6CMP0
C	1440	TRP	-	expression tag	UNP A0A8E6CMP0
C	1441	HIS	-	expression tag	UNP A0A8E6CMP0
C	1442	GLU	-	expression tag	UNP A0A8E6CMP0
C	1443	GLY	-	expression tag	UNP A0A8E6CMP0
C	1444	GLY	-	expression tag	UNP A0A8E6CMP0
C	1445	SER	-	expression tag	UNP A0A8E6CMP0
C	1446	HIS	-	expression tag	UNP A0A8E6CMP0
C	1447	HIS	-	expression tag	UNP A0A8E6CMP0
C	1448	HIS	-	expression tag	UNP A0A8E6CMP0
C	1449	HIS	-	expression tag	UNP A0A8E6CMP0
C	1450	HIS	-	expression tag	UNP A0A8E6CMP0
C	1451	HIS	-	expression tag	UNP A0A8E6CMP0
C	1452	HIS	-	expression tag	UNP A0A8E6CMP0
C	1453	HIS	-	expression tag	UNP A0A8E6CMP0

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

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

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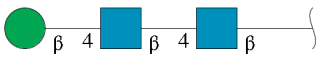
Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		

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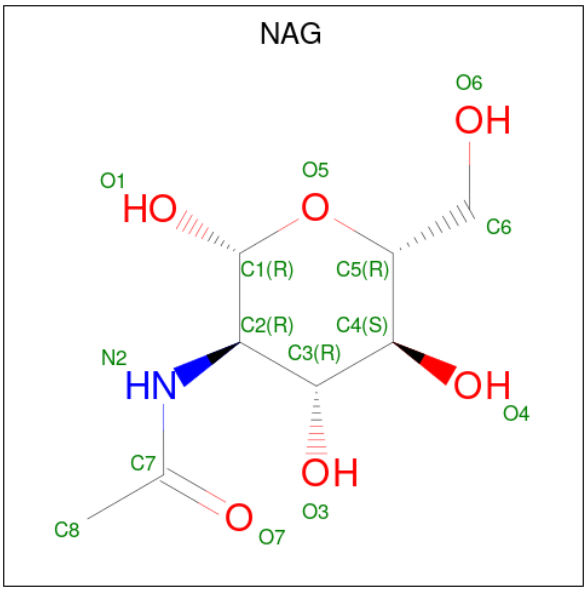
Mol	Chain	Residues	Atoms	AltConf	Trace
3	S	3	Total C N O 39 22 2 15	0	0
3	U	3	Total C N O 39 22 2 15	0	0
3	b	3	Total C N O 39 22 2 15	0	0
3	d	3	Total C N O 39 22 2 15	0	0

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



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

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

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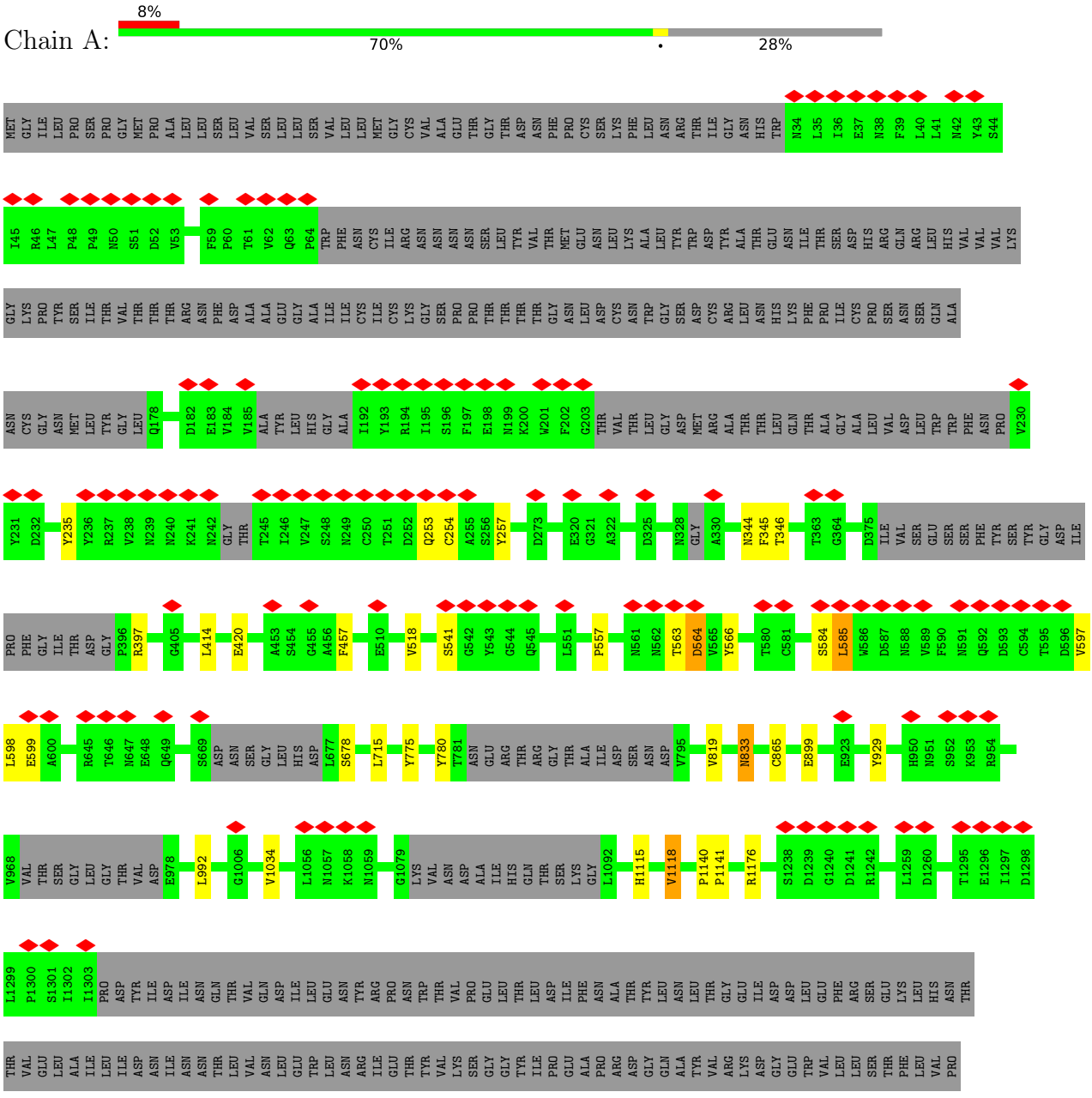
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			140	80	10	50	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

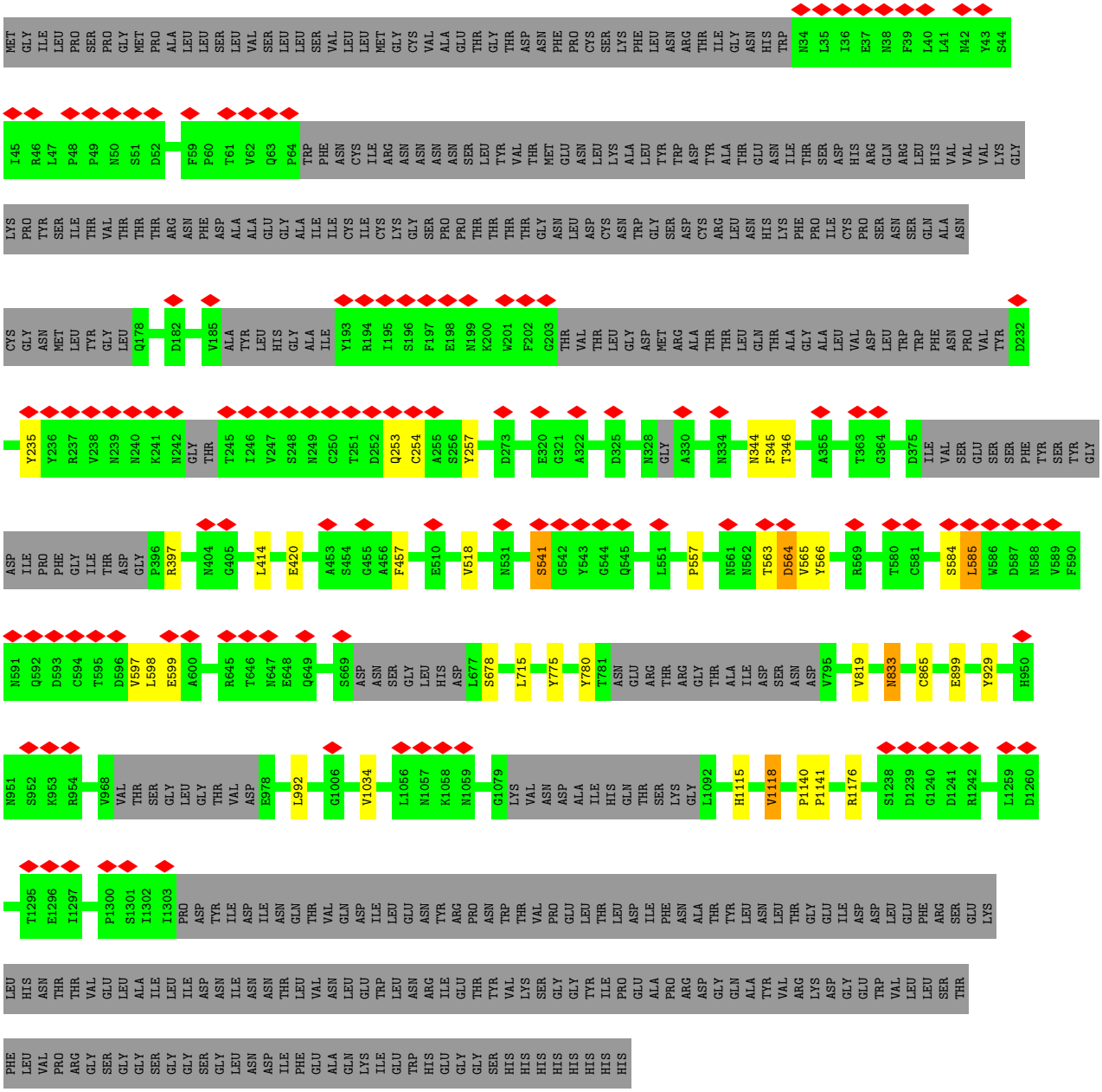
- Molecule 1: Spike glycoprotein

Chain A:



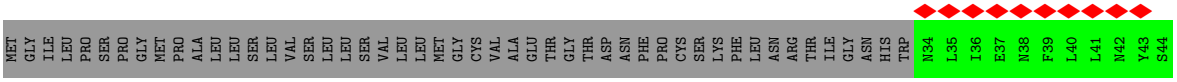
• Molecule 1: Spike glycoprotein

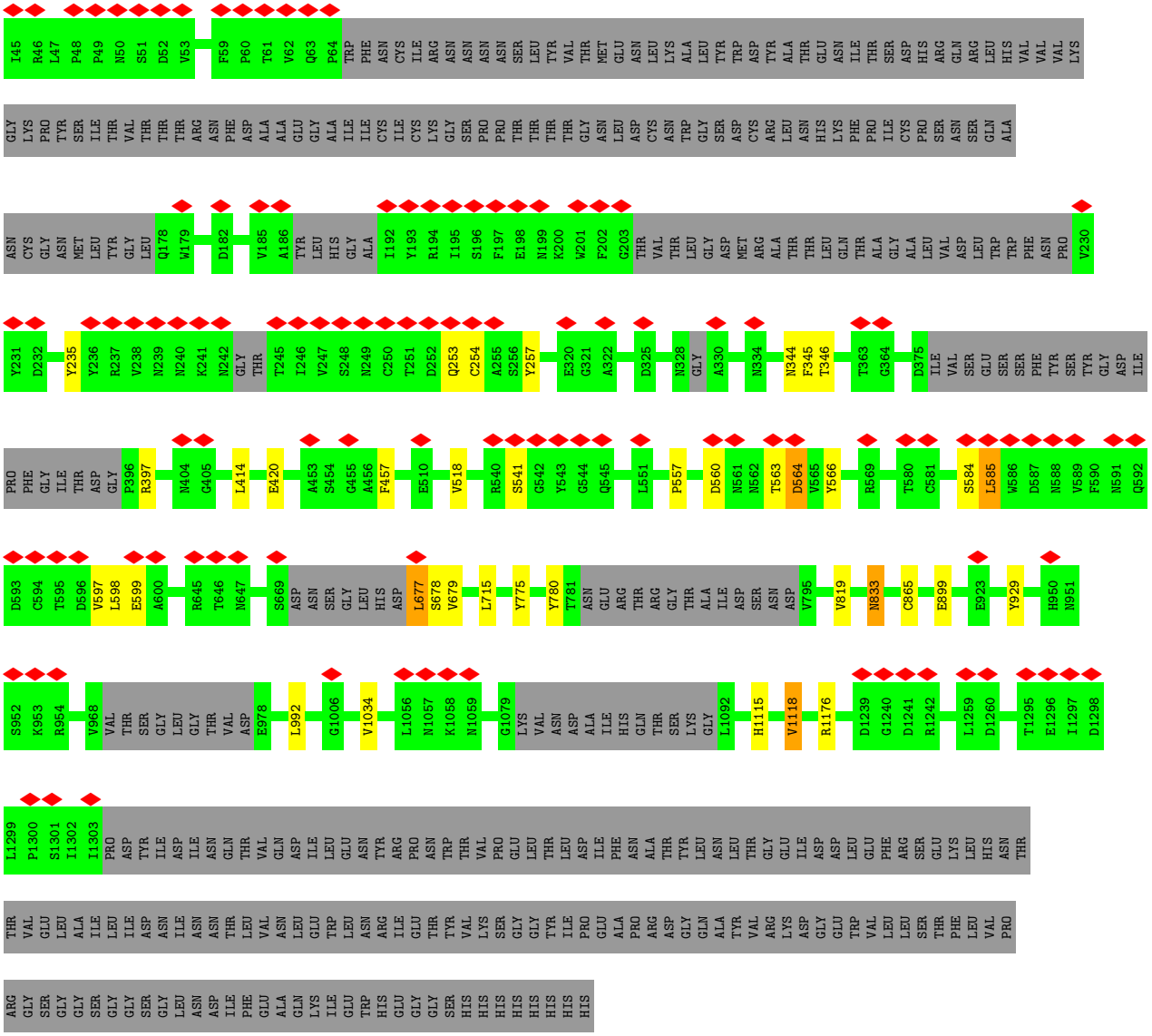
Chain B:



• Molecule 1: Spike glycoprotein

Chain C:



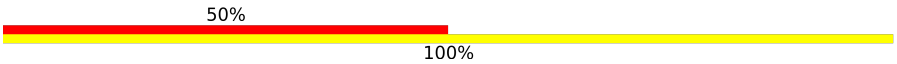


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

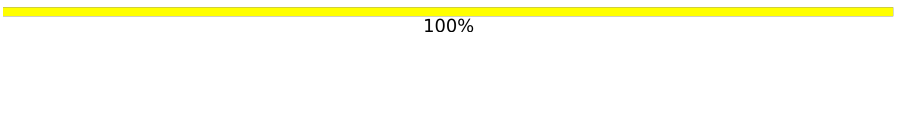
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



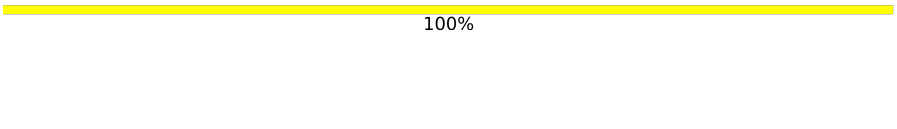
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



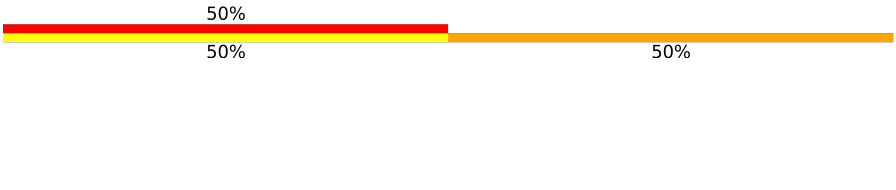
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



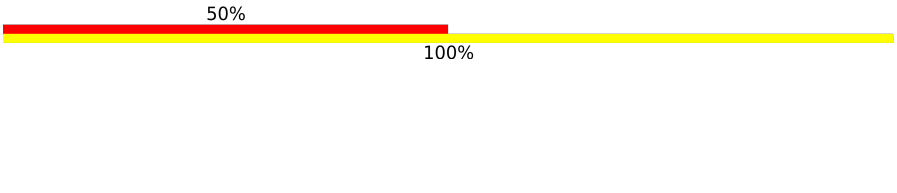
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



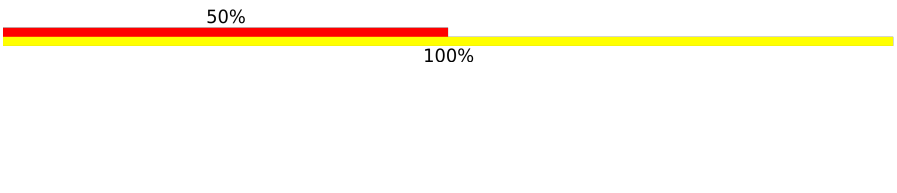
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



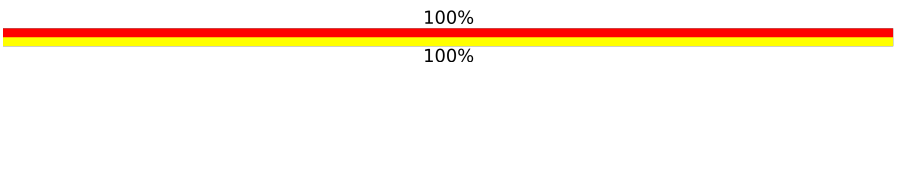
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



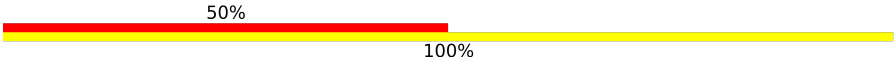
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



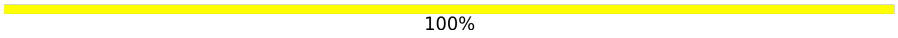
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



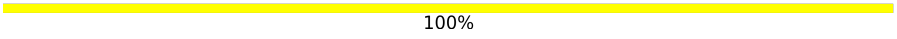
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain P:



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

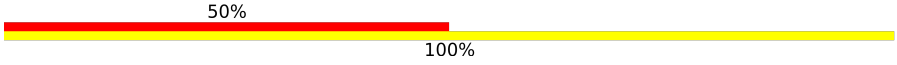
Chain Q:

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

Chain R:

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

Chain T:



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

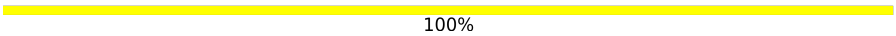
Chain V:

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

Chain W:

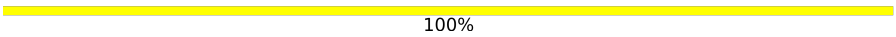
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain Y:

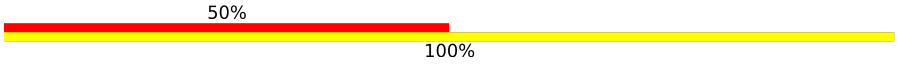


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

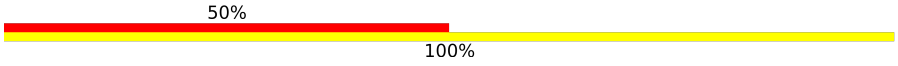
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



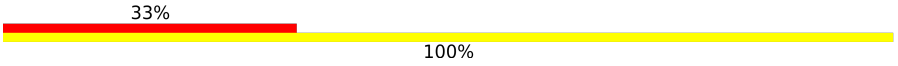
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



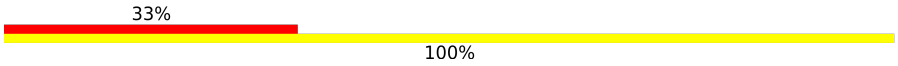
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



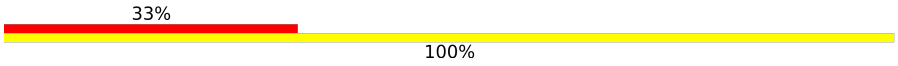
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



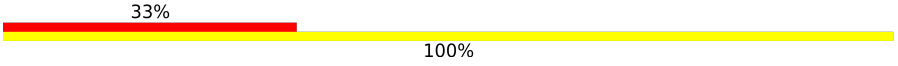
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



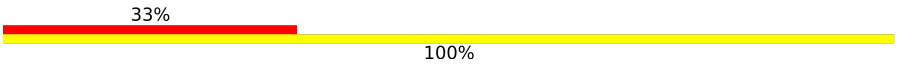
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



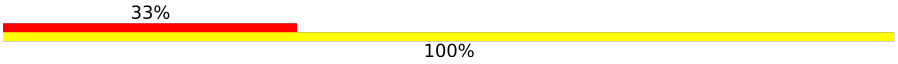
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



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

Chain d:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.425	Depositor
Minimum map value	-3.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.706	Depositor
Map size (Å)	431.616, 431.616, 431.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.68	2/7849 (0.0%)	0.78	13/10741 (0.1%)
1	B	0.68	2/7835 (0.0%)	0.77	13/10723 (0.1%)
1	C	0.68	2/7850 (0.0%)	0.77	13/10745 (0.1%)
All	All	0.68	6/23534 (0.0%)	0.77	39/32209 (0.1%)

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

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	865	CYS	C-O	6.09	1.34	1.23
1	B	865	CYS	C-O	6.07	1.34	1.23
1	C	865	CYS	C-O	6.06	1.34	1.23
1	A	420	GLU	CD-OE1	-5.67	1.19	1.25
1	B	420	GLU	CD-OE1	-5.62	1.19	1.25

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	585	LEU	N-CA-CB	15.25	140.89	110.40
1	A	585	LEU	N-CA-CB	15.23	140.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	585	LEU	N-CA-CB	15.23	140.85	110.40
1	C	584	SER	N-CA-C	13.32	146.97	111.00
1	B	584	SER	N-CA-C	13.32	146.96	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	833	ASN	Mainchain
1	B	833	ASN	Mainchain
1	C	833	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7694	0	7149	30	0
1	B	7678	0	7101	31	0
1	C	7693	0	7108	32	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	T	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	28	0	25	1	0
2	a	28	0	25	0	0
2	c	28	0	25	0	0
3	J	39	0	34	0	0
3	L	39	0	34	0	0
3	S	39	0	34	0	0
3	U	39	0	34	0	0
3	b	39	0	34	0	0
3	d	39	0	34	0	0
4	A	140	0	130	0	0
4	B	140	0	130	0	0
4	C	140	0	130	0	0
All	All	24307	0	22477	86	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 2.

The worst 5 of 86 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TYR:HE2	1:B:457:PHE:CZ	1.46	1.34
1:C:235:TYR:HE2	1:C:457:PHE:CZ	1.46	1.33
1:A:235:TYR:HE2	1:A:457:PHE:CZ	1.46	1.33
1:C:235:TYR:CE2	1:C:457:PHE:CZ	2.26	1.23
1:A:235:TYR:CE2	1:A:457:PHE:CZ	2.26	1.22

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	1039/1469 (71%)	999 (96%)	37 (4%)	3 (0%)	41 72
1	B	1036/1469 (70%)	997 (96%)	36 (4%)	3 (0%)	41 72
1	C	1040/1469 (71%)	1001 (96%)	36 (4%)	3 (0%)	41 72
All	All	3115/4407 (71%)	2997 (96%)	109 (4%)	9 (0%)	44 72

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	LEU
1	B	585	LEU
1	C	585	LEU
1	A	564	ASP
1	B	564	ASP

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	763/1269 (60%)	763 (100%)	0	100 100
1	B	766/1269 (60%)	766 (100%)	0	100 100
1	C	764/1269 (60%)	763 (100%)	1 (0%)	93 98
All	All	2293/3807 (60%)	2292 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	677	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1107	ASN
1	A	1164	GLN

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Mol	Chain	Res	Type
1	B	1107	ASN
1	C	1107	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)

60 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	1.46	2 (14%)	17,19,21	1.07	1 (5%)
2	NAG	D	2	2	14,14,15	1.42	2 (14%)	17,19,21	0.89	1 (5%)
2	NAG	E	1	2,1	14,14,15	1.49	2 (14%)	17,19,21	0.94	1 (5%)
2	NAG	E	2	2	14,14,15	1.43	2 (14%)	17,19,21	0.82	1 (5%)
2	NAG	F	1	2,1	14,14,15	1.36	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	F	2	2	14,14,15	1.35	2 (14%)	17,19,21	0.80	0
2	NAG	G	1	2,1	14,14,15	1.42	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	G	2	2	14,14,15	1.39	2 (14%)	17,19,21	0.93	1 (5%)
2	NAG	H	1	2,1	14,14,15	1.86	3 (21%)	17,19,21	0.86	0
2	NAG	H	2	2	14,14,15	1.90	4 (28%)	17,19,21	1.69	4 (23%)
2	NAG	I	1	2,1	14,14,15	1.50	1 (7%)	17,19,21	0.91	0
2	NAG	I	2	2	14,14,15	1.42	2 (14%)	17,19,21	0.95	1 (5%)
3	NAG	J	1	3,1	14,14,15	2.16	4 (28%)	17,19,21	2.46	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	J	2	3	14,14,15	0.53	0	17,19,21	1.39	1 (5%)
3	BMA	J	3	3	11,11,12	1.42	3 (27%)	15,15,17	0.70	0
2	NAG	K	1	2,1	14,14,15	1.62	2 (14%)	17,19,21	1.43	2 (11%)
2	NAG	K	2	2	14,14,15	1.44	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	L	1	3,1	14,14,15	1.61	1 (7%)	17,19,21	1.69	4 (23%)
3	NAG	L	2	3	14,14,15	0.50	0	17,19,21	1.28	1 (5%)
3	BMA	L	3	3	11,11,12	1.51	4 (36%)	15,15,17	0.68	0
2	NAG	M	1	2,1	14,14,15	1.46	2 (14%)	17,19,21	1.07	1 (5%)
2	NAG	M	2	2	14,14,15	1.41	2 (14%)	17,19,21	0.88	1 (5%)
2	NAG	N	1	2,1	14,14,15	1.49	2 (14%)	17,19,21	0.94	1 (5%)
2	NAG	N	2	2	14,14,15	1.43	2 (14%)	17,19,21	0.82	1 (5%)
2	NAG	O	1	2,1	14,14,15	1.36	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	O	2	2	14,14,15	1.35	2 (14%)	17,19,21	0.80	0
2	NAG	P	1	2,1	14,14,15	1.42	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	P	2	2	14,14,15	1.39	2 (14%)	17,19,21	0.93	1 (5%)
2	NAG	Q	1	2,1	14,14,15	1.86	3 (21%)	17,19,21	0.86	0
2	NAG	Q	2	2	14,14,15	1.89	4 (28%)	17,19,21	1.68	4 (23%)
2	NAG	R	1	2,1	14,14,15	1.49	1 (7%)	17,19,21	0.91	0
2	NAG	R	2	2	14,14,15	1.42	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	S	1	3,1	14,14,15	2.16	4 (28%)	17,19,21	2.46	5 (29%)
3	NAG	S	2	3	14,14,15	0.53	0	17,19,21	1.39	1 (5%)
3	BMA	S	3	3	11,11,12	1.42	3 (27%)	15,15,17	0.70	0
2	NAG	T	1	2,1	14,14,15	1.60	2 (14%)	17,19,21	1.43	2 (11%)
2	NAG	T	2	2	14,14,15	1.45	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	U	1	3,1	14,14,15	1.61	1 (7%)	17,19,21	1.69	4 (23%)
3	NAG	U	2	3	14,14,15	0.49	0	17,19,21	1.28	1 (5%)
3	BMA	U	3	3	11,11,12	1.51	4 (36%)	15,15,17	0.68	0
2	NAG	V	1	2,1	14,14,15	1.46	2 (14%)	17,19,21	1.07	1 (5%)
2	NAG	V	2	2	14,14,15	1.41	2 (14%)	17,19,21	0.89	1 (5%)
2	NAG	W	1	2,1	14,14,15	1.49	2 (14%)	17,19,21	0.94	1 (5%)
2	NAG	W	2	2	14,14,15	1.43	2 (14%)	17,19,21	0.82	1 (5%)
2	NAG	X	1	2,1	14,14,15	1.35	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	X	2	2	14,14,15	1.35	2 (14%)	17,19,21	0.80	0
2	NAG	Y	1	2,1	14,14,15	1.43	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	Y	2	2	14,14,15	1.39	2 (14%)	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	Z	1	2,1	14,14,15	1.86	3 (21%)	17,19,21	0.86	0
2	NAG	Z	2	2	14,14,15	1.90	4 (28%)	17,19,21	1.69	4 (23%)
2	NAG	a	1	2,1	14,14,15	1.49	1 (7%)	17,19,21	0.91	0
2	NAG	a	2	2	14,14,15	1.42	2 (14%)	17,19,21	0.95	1 (5%)
3	NAG	b	1	3,1	14,14,15	2.15	4 (28%)	17,19,21	2.46	5 (29%)
3	NAG	b	2	3	14,14,15	0.52	0	17,19,21	1.39	1 (5%)
3	BMA	b	3	3	11,11,12	1.41	3 (27%)	15,15,17	0.70	0
2	NAG	c	1	2,1	14,14,15	1.61	2 (14%)	17,19,21	1.44	2 (11%)
2	NAG	c	2	2	14,14,15	1.44	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	d	1	3,1	14,14,15	1.61	1 (7%)	17,19,21	1.69	4 (23%)
3	NAG	d	2	3	14,14,15	0.49	0	17,19,21	1.28	1 (5%)
3	BMA	d	3	3	11,11,12	1.51	4 (36%)	15,15,17	0.68	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1
2	NAG	V	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	3/6/23/26	0/1/1/1
2	NAG	a	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
3	NAG	b	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	BMA	b	3	3	-	2/2/19/22	0/1/1/1
2	NAG	c	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
3	NAG	d	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	BMA	d	3	3	-	2/2/19/22	0/1/1/1

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	C1-C2	6.38	1.61	1.52
3	S	1	NAG	C1-C2	6.37	1.61	1.52
3	b	1	NAG	C1-C2	6.36	1.61	1.52
2	H	2	NAG	C1-C2	5.24	1.60	1.52
2	Z	2	NAG	C1-C2	5.24	1.60	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1	NAG	C8-C7-N2	5.44	125.31	116.10
3	S	1	NAG	C8-C7-N2	5.44	125.31	116.10
3	b	1	NAG	C8-C7-N2	5.42	125.28	116.10
3	L	1	NAG	C2-N2-C7	5.01	130.03	122.90
3	U	1	NAG	C2-N2-C7	5.00	130.03	122.90

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	Z	1	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2

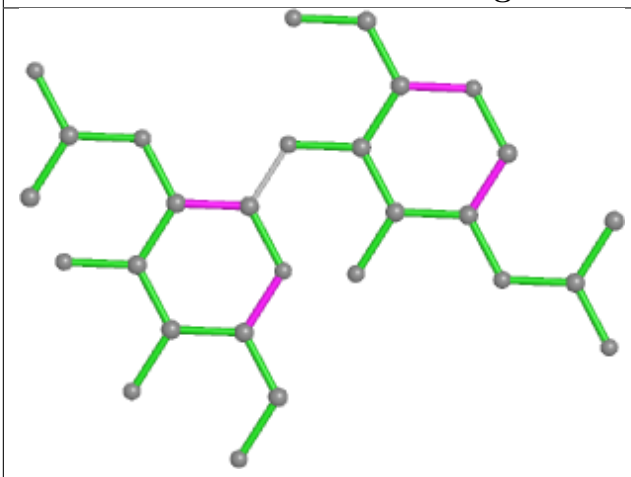
There are no ring outliers.

3 monomers are involved in 3 short contacts:

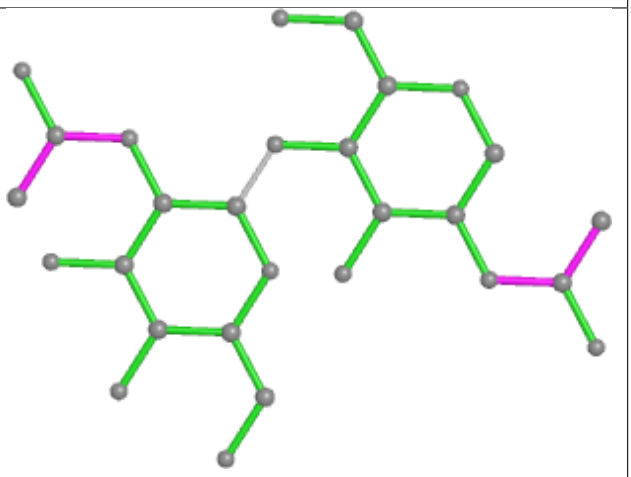
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	1	0
2	H	1	NAG	1	0
2	Z	1	NAG	1	0

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

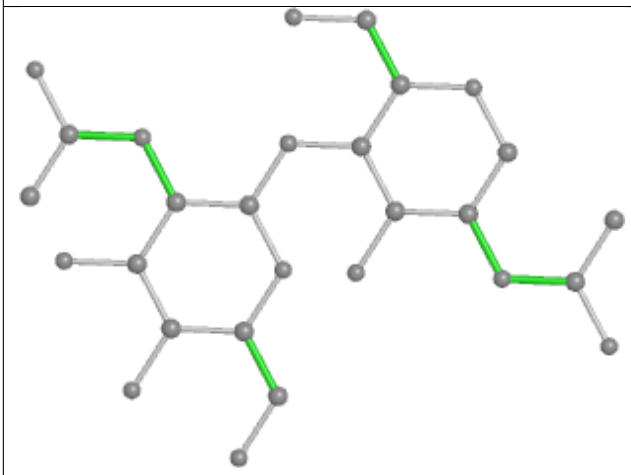
Oligosaccharide Chain D



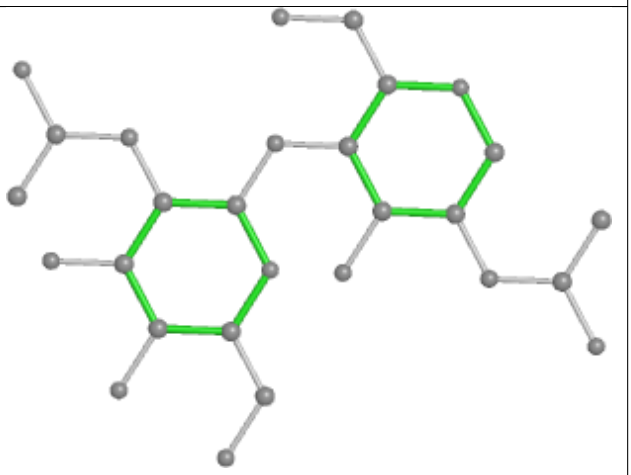
Bond lengths



Bond angles

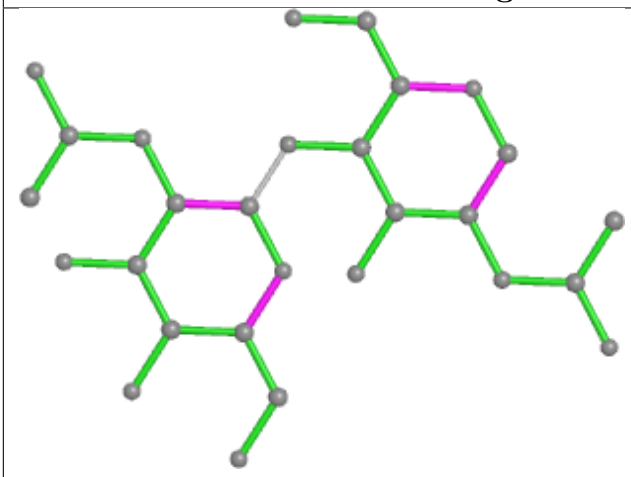


Torsions

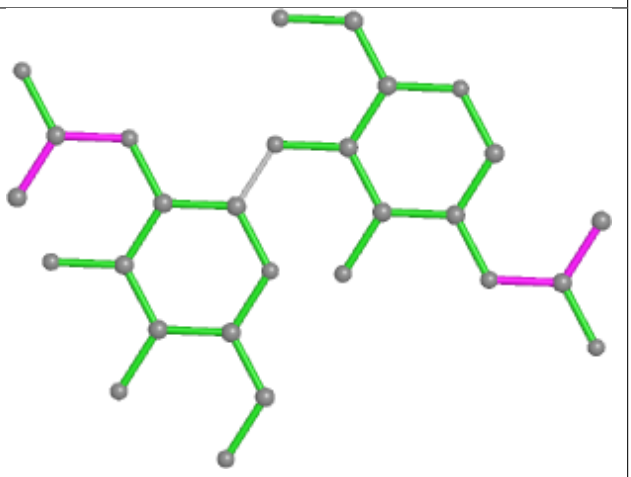


Rings

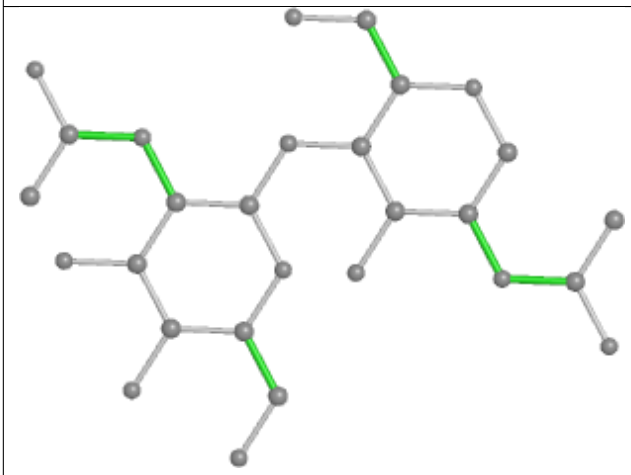
Oligosaccharide Chain E



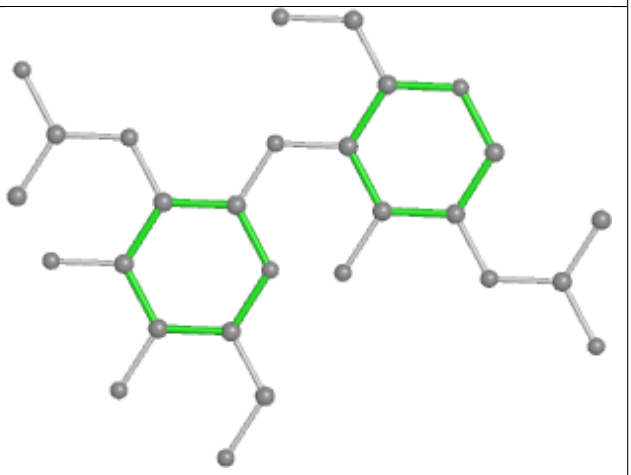
Bond lengths



Bond angles

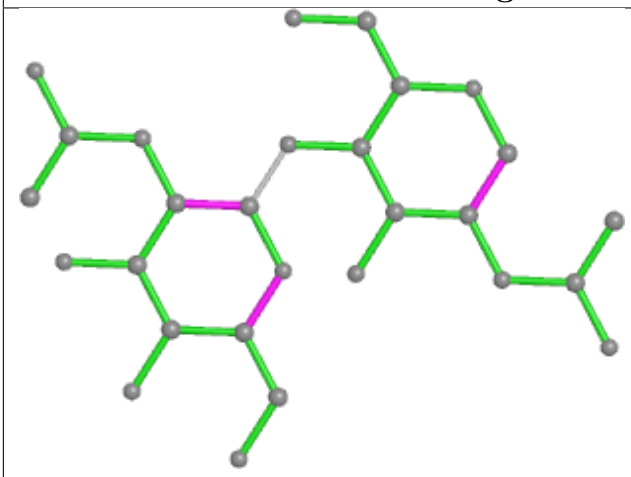


Torsions



Rings

Oligosaccharide Chain F



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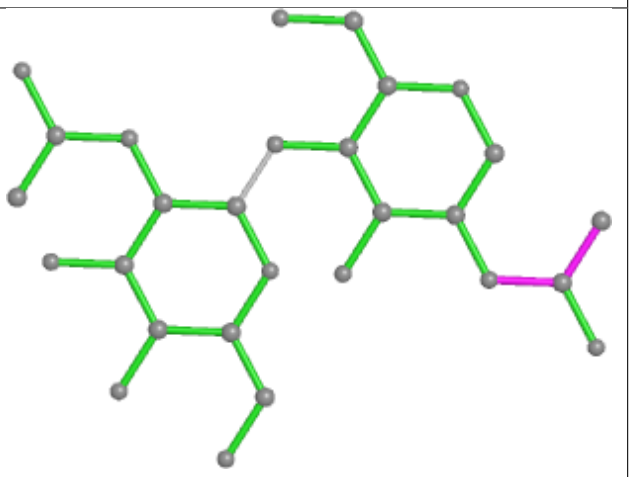
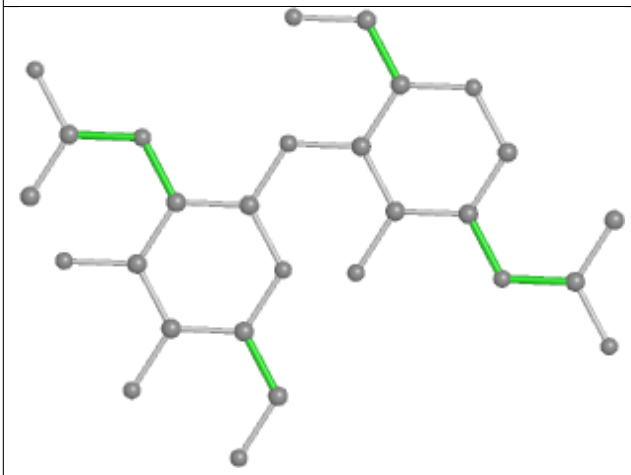
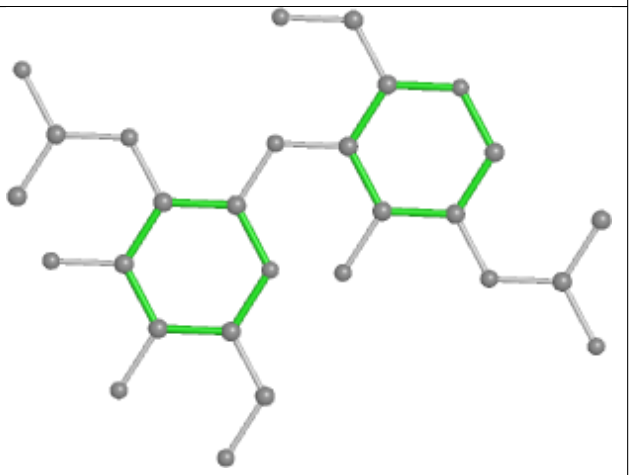


Bond angles

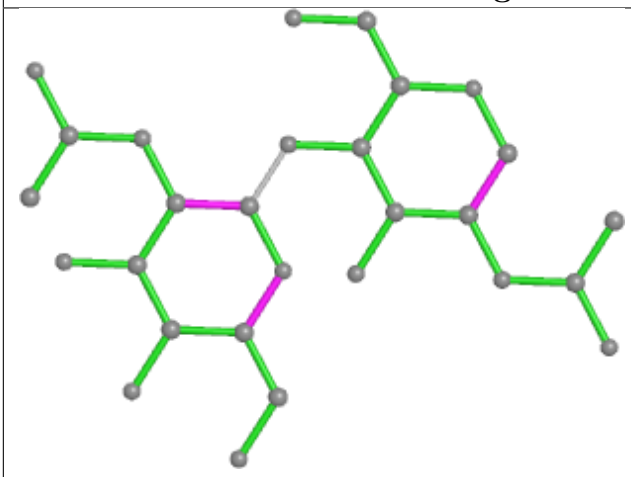


Torsions

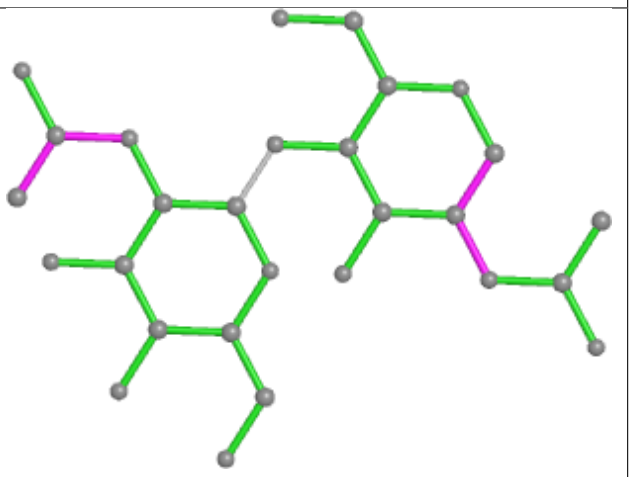


Rings

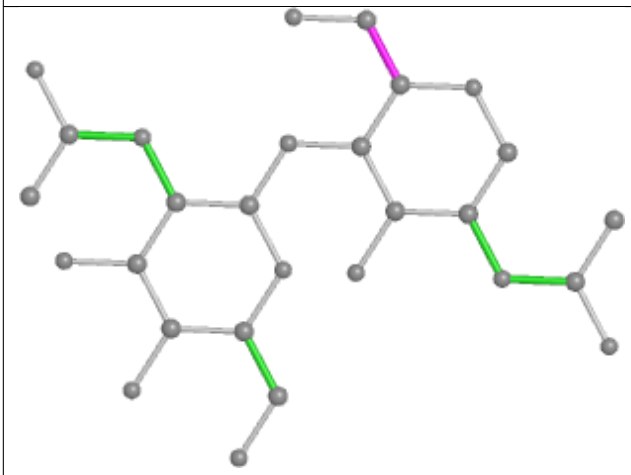
Oligosaccharide Chain G



Bond lengths



Bond angles



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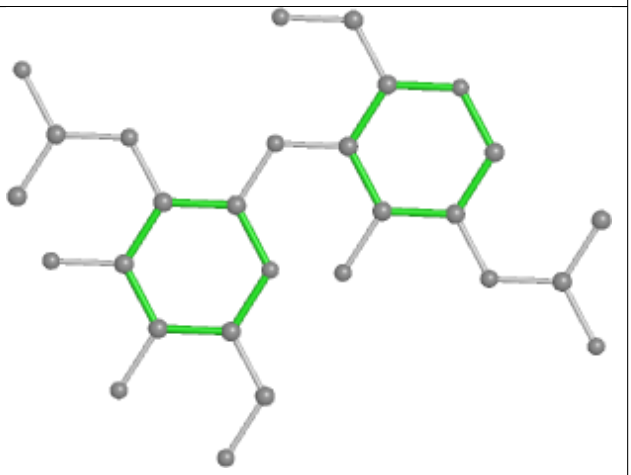
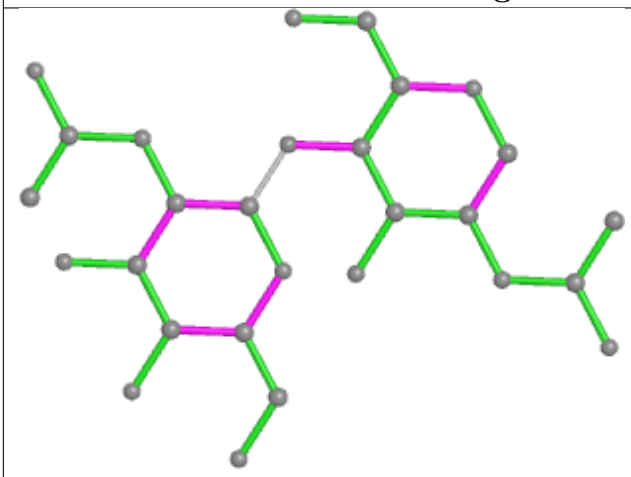


Rings

Oligosaccharide Chain H



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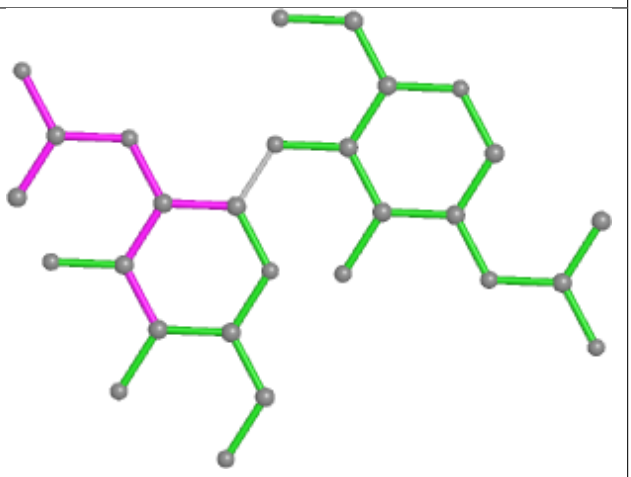

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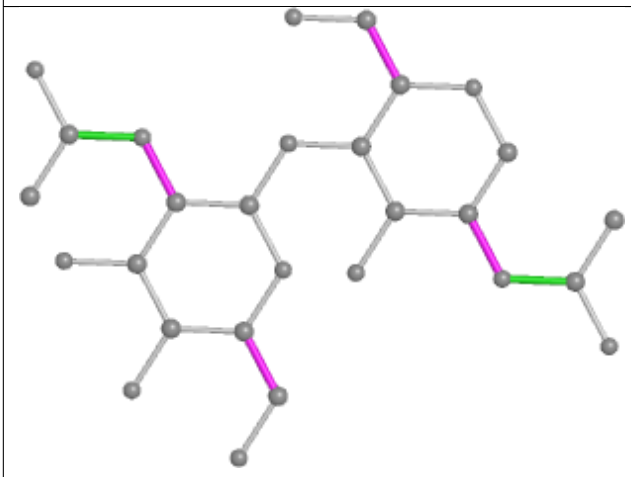

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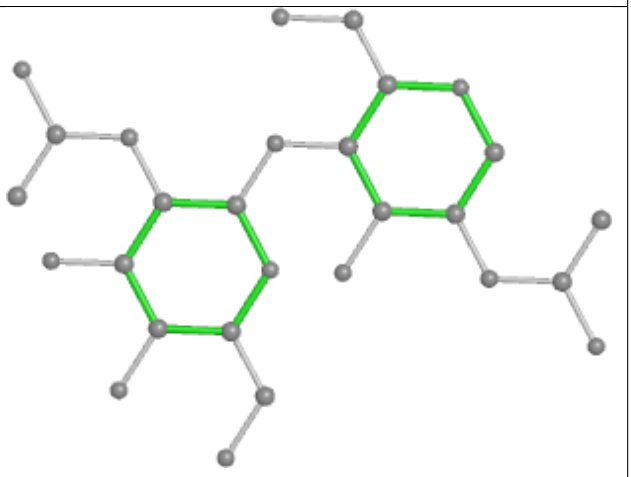
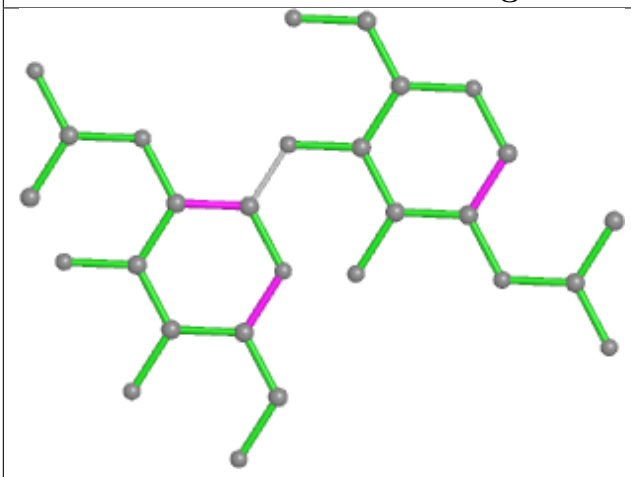


Rings

Oligosaccharide Chain I



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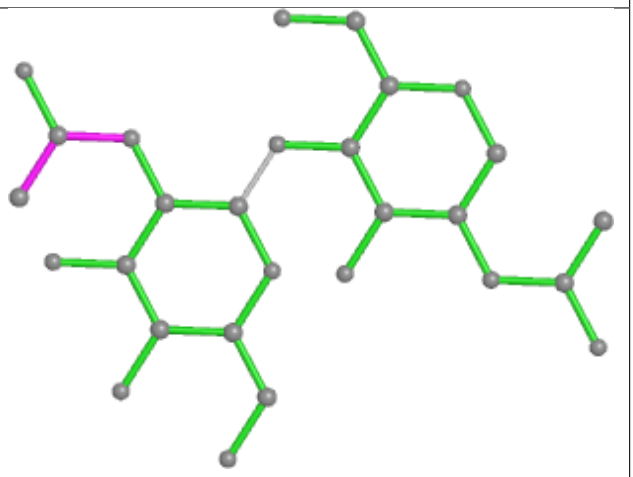

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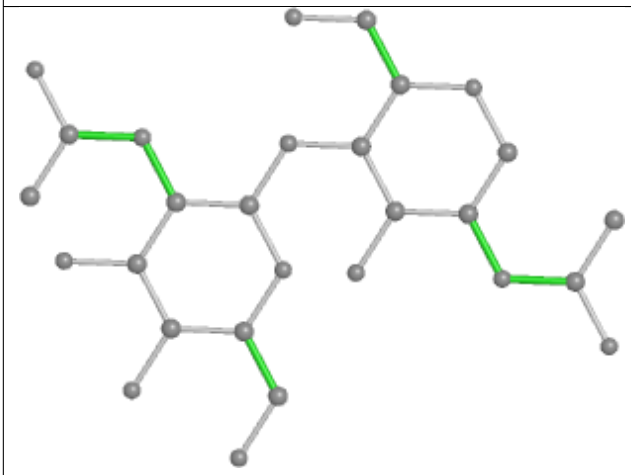

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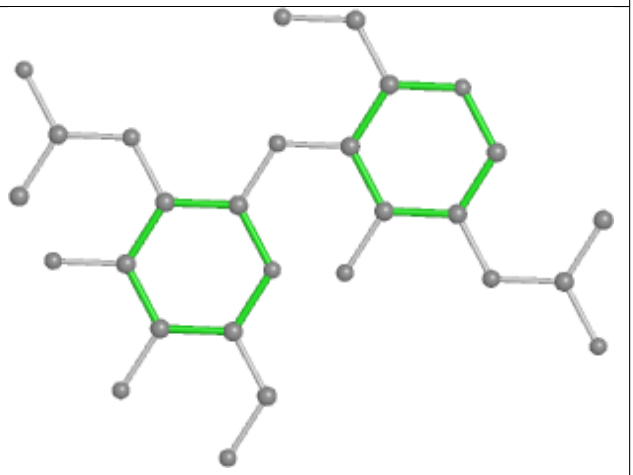
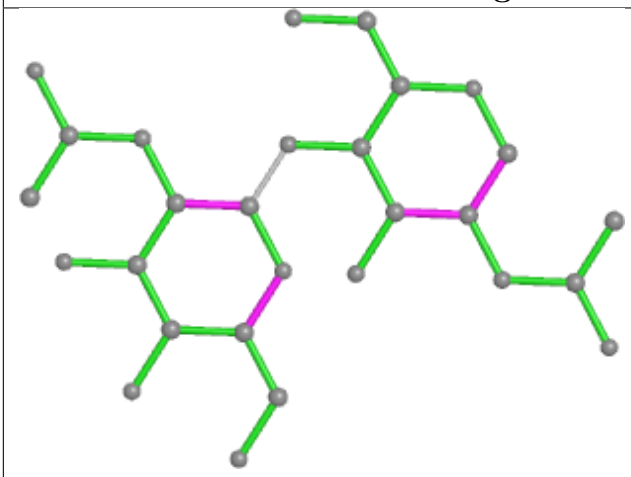


Rings

Oligosaccharide Chain K



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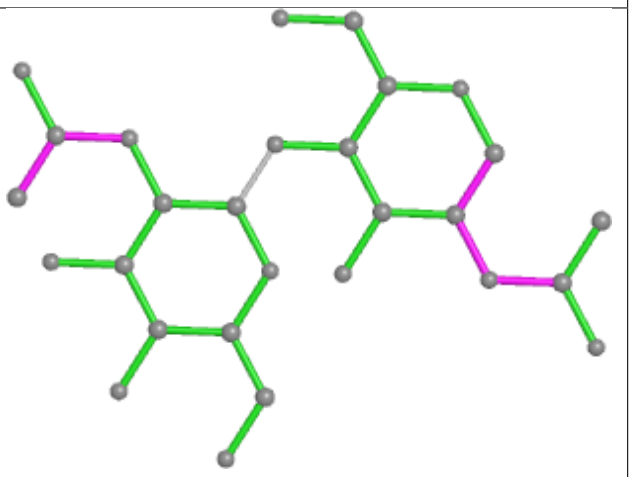
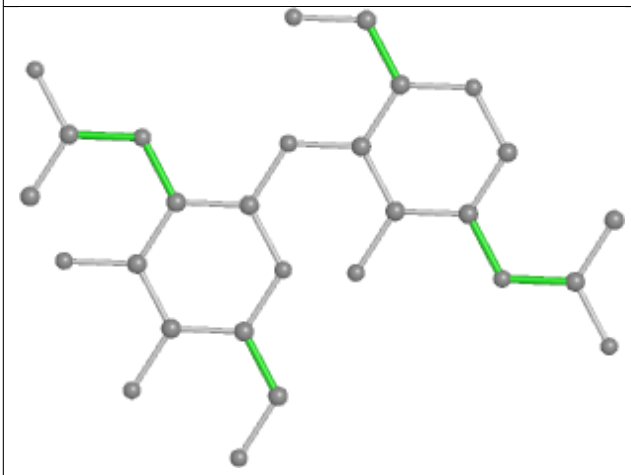


Bond angles



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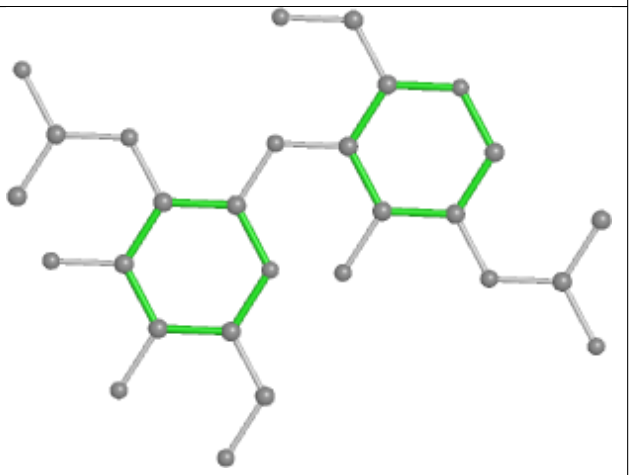
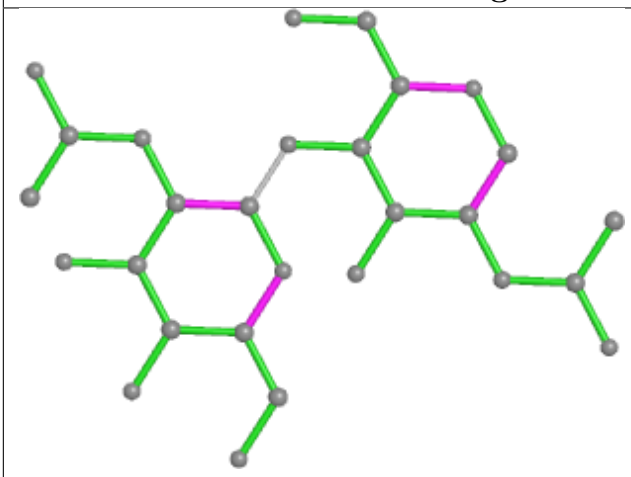


Rings

Oligosaccharide Chain M



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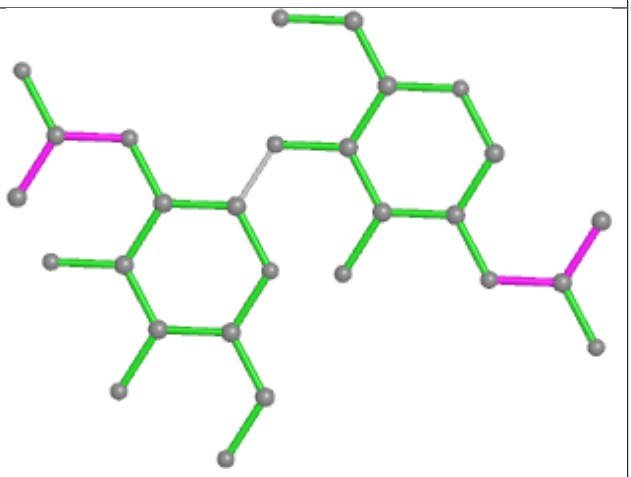
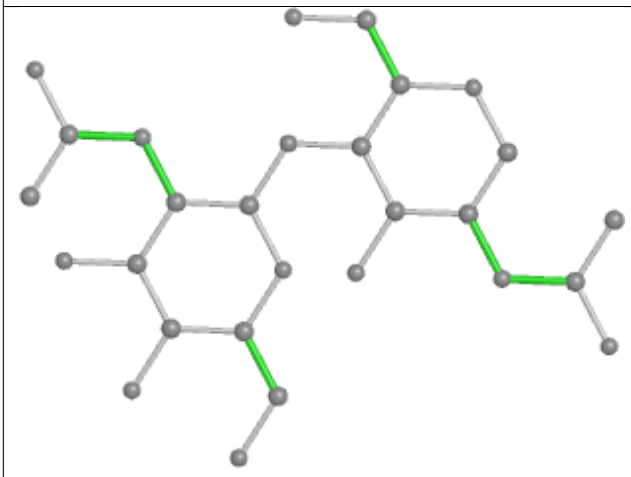


Bond angles



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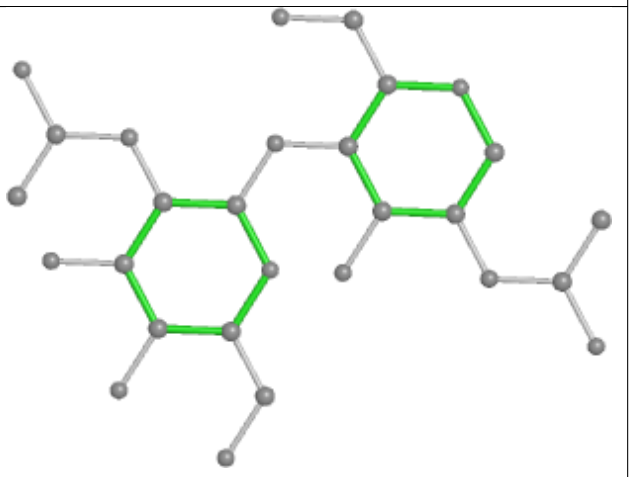
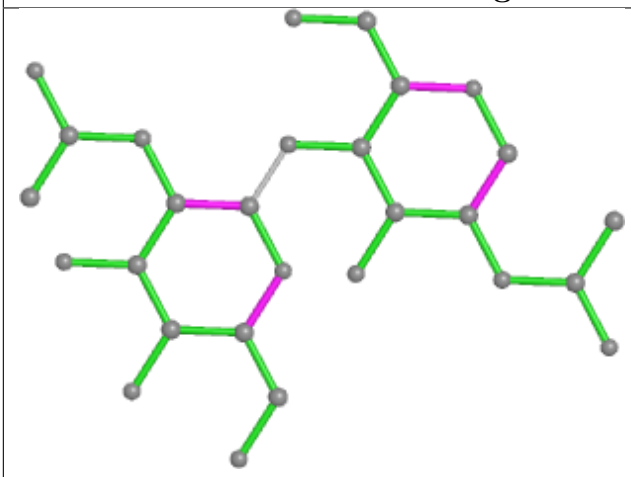
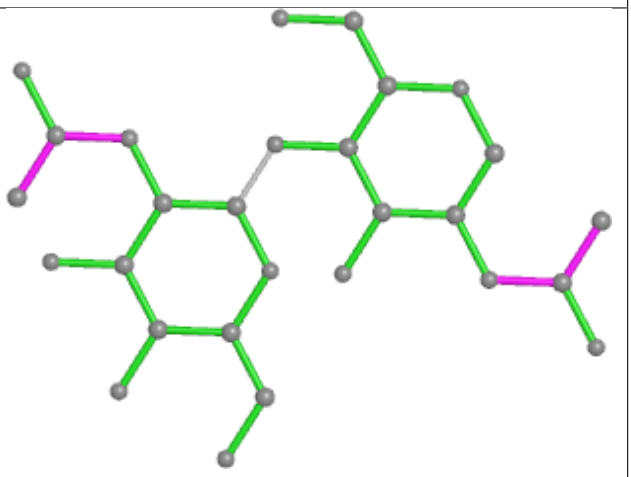
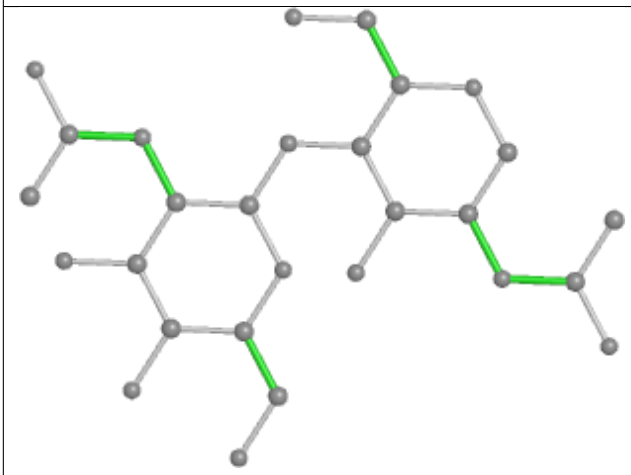
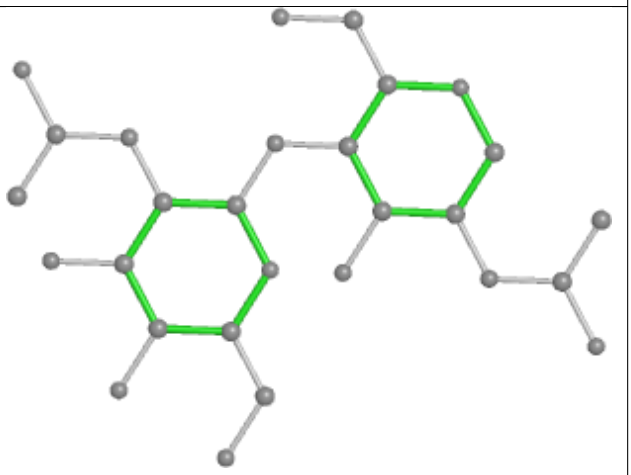
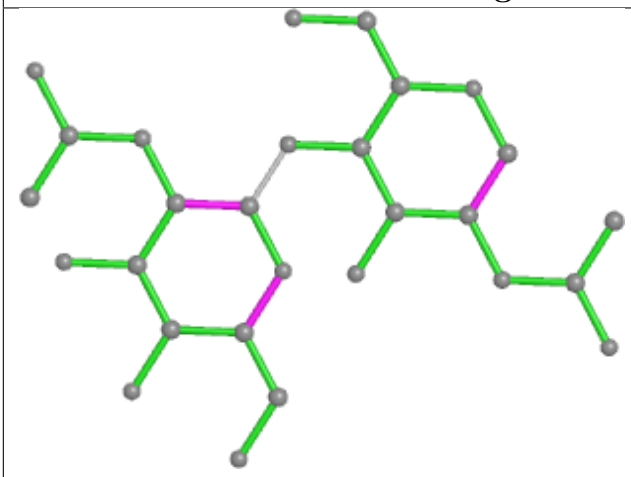


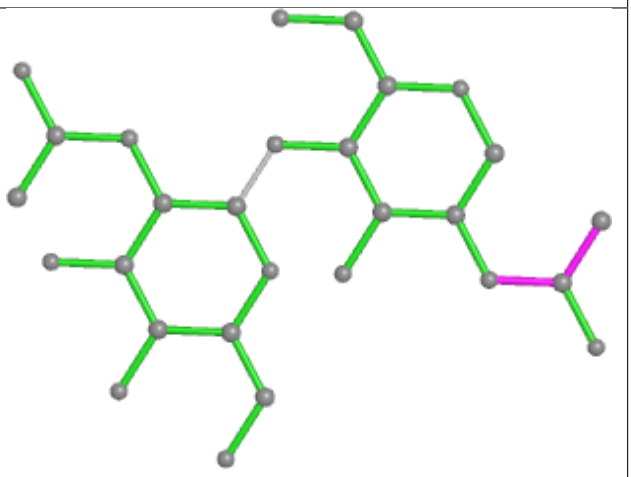
Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

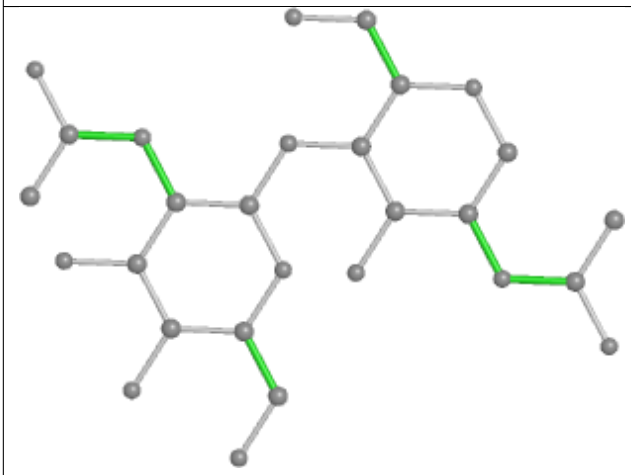
Oligosaccharide Chain O



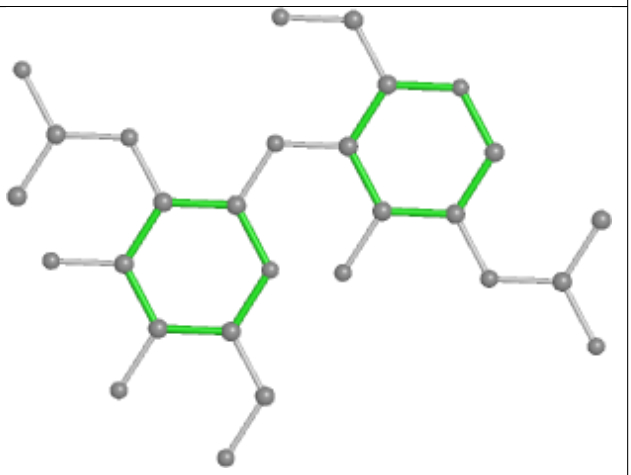
Bond lengths



Bond angles

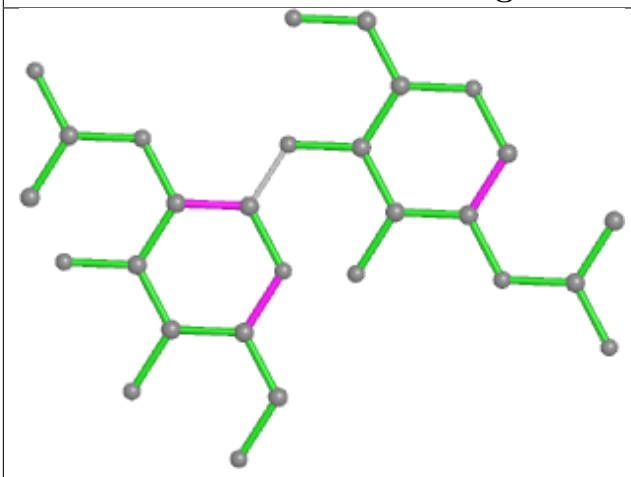


Torsions

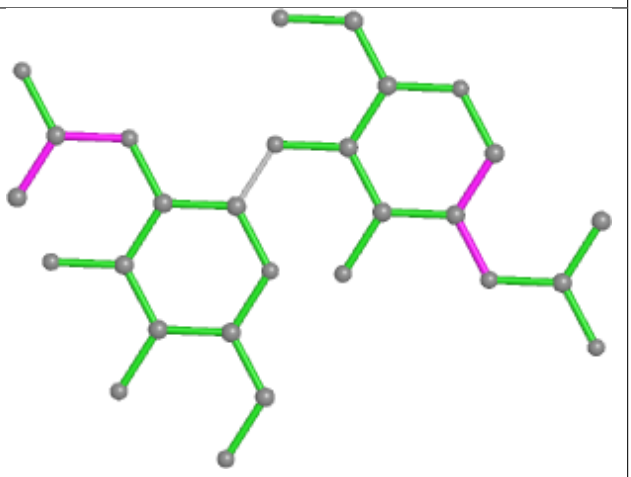


Rings

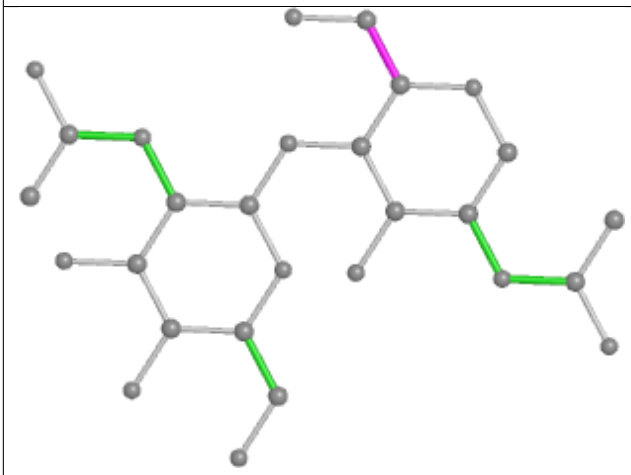
Oligosaccharide Chain P



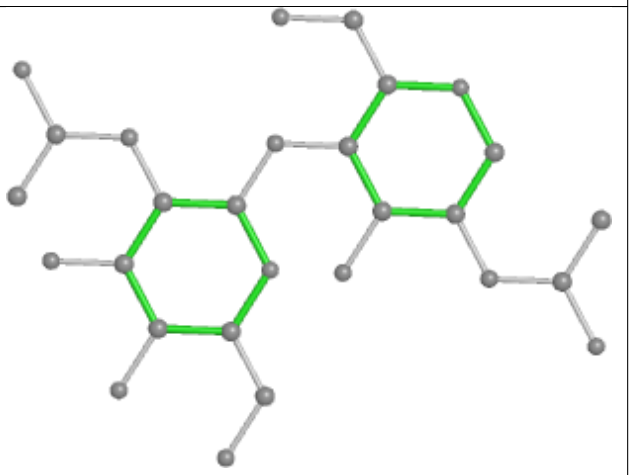
Bond lengths



Bond angles

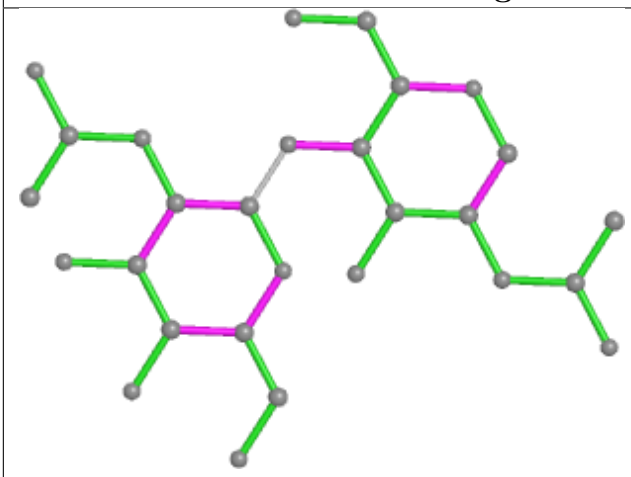


Torsions

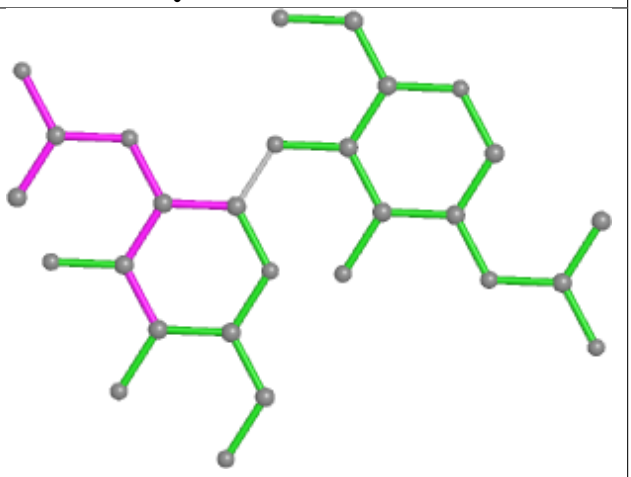


Rings

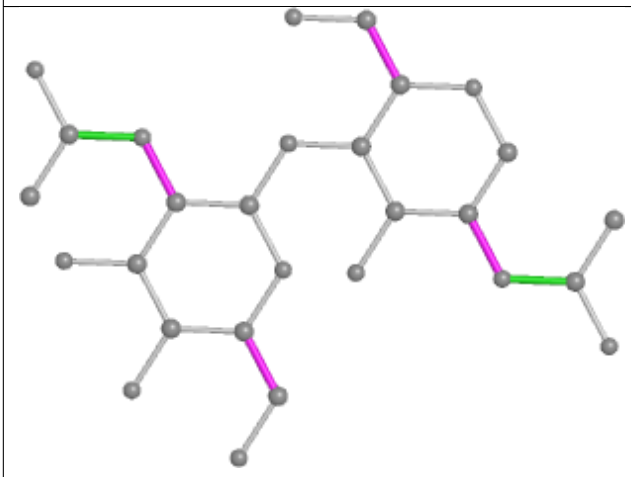
Oligosaccharide Chain Q



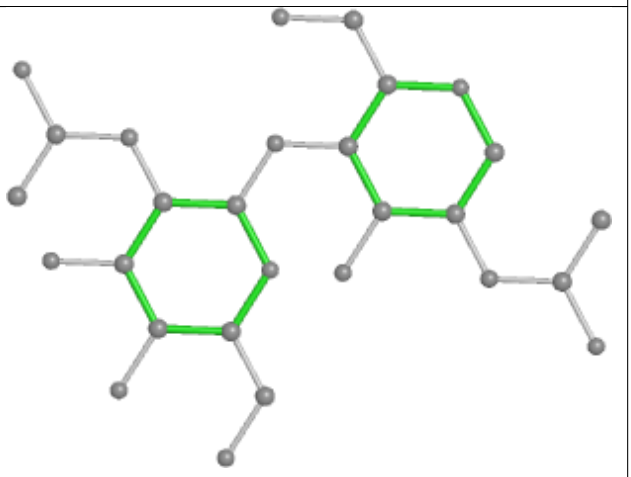
Bond lengths



Bond angles

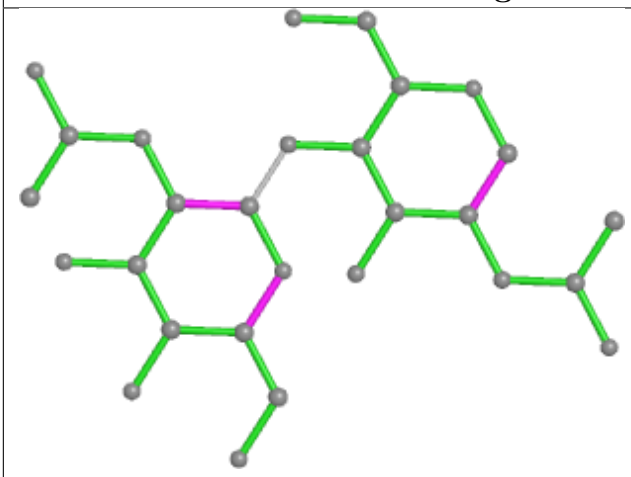


Torsions

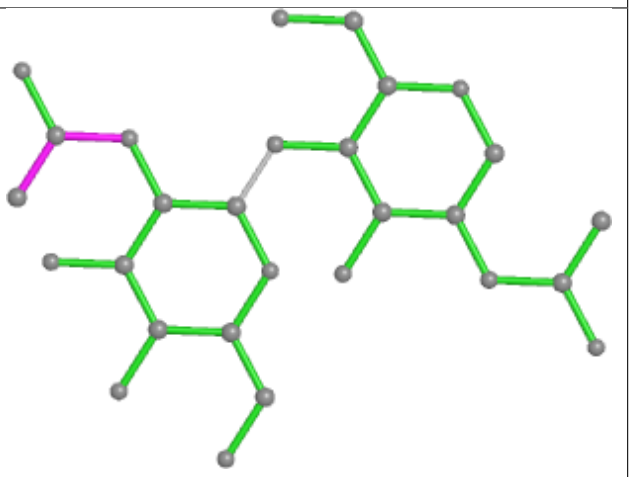


Rings

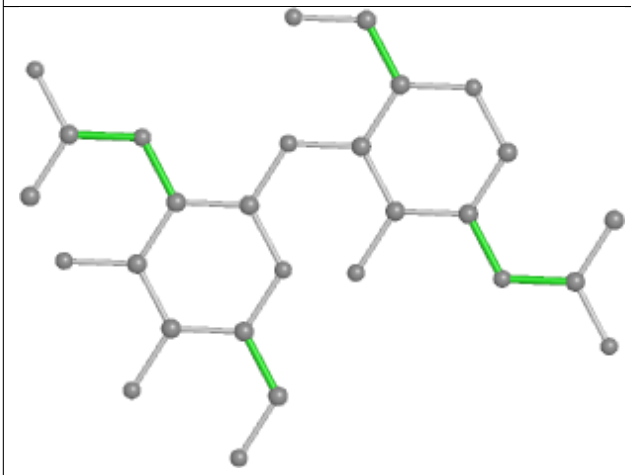
Oligosaccharide Chain R



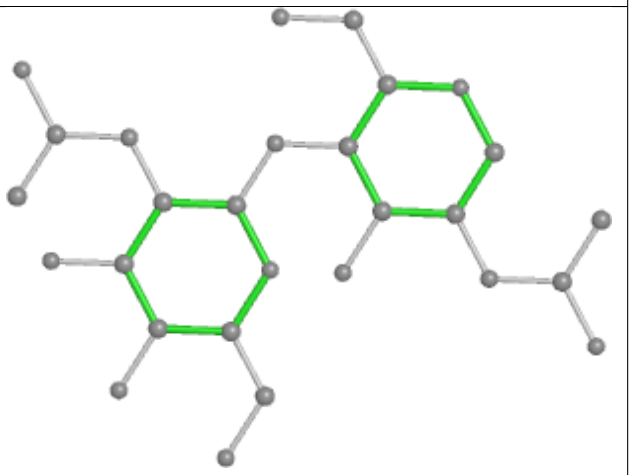
Bond lengths



Bond angles

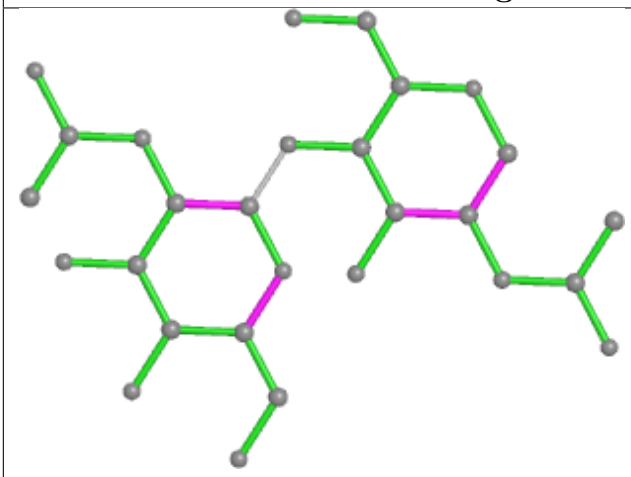


Torsions



Rings

Oligosaccharide Chain T



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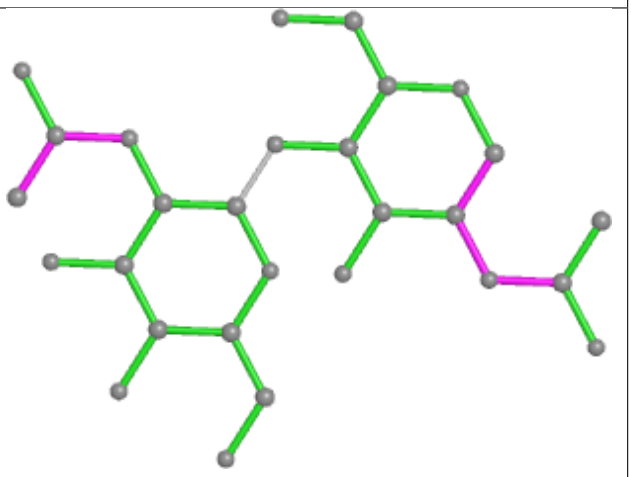
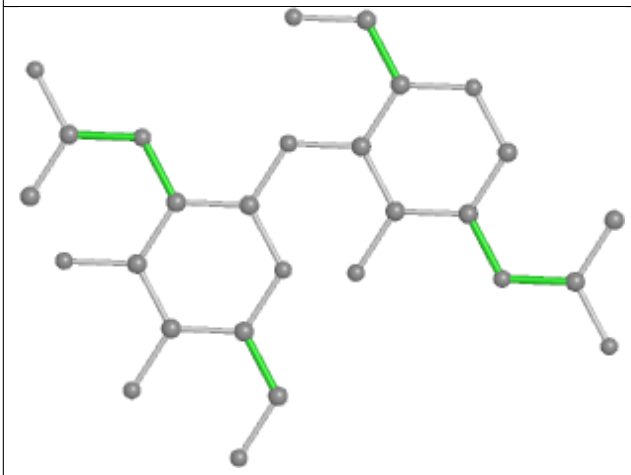
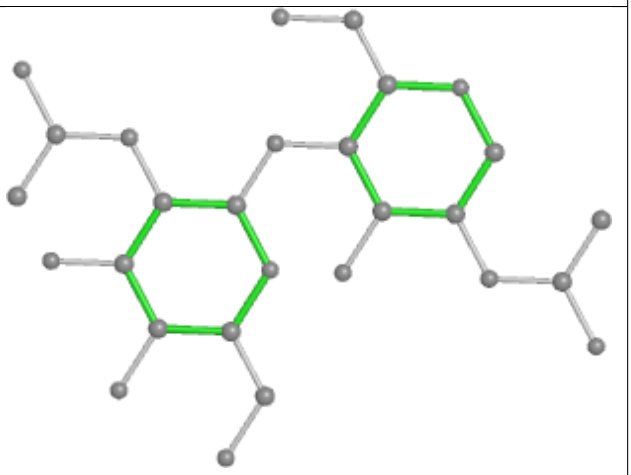


Bond angles

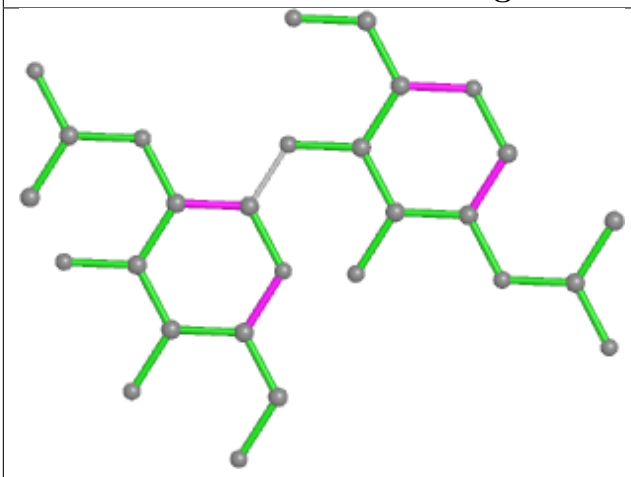


Torsions



Rings

Oligosaccharide Chain V



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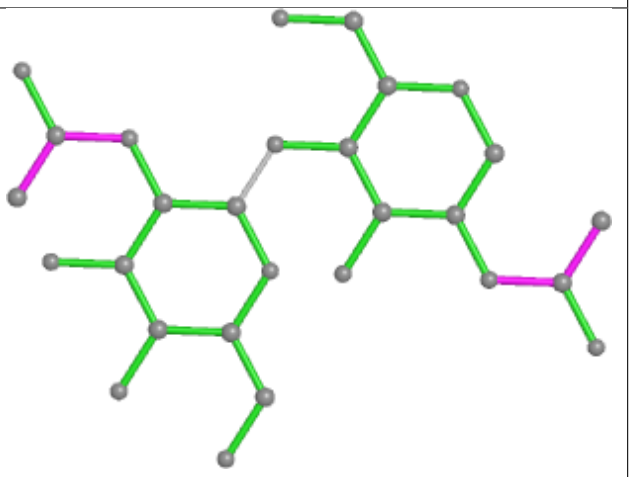
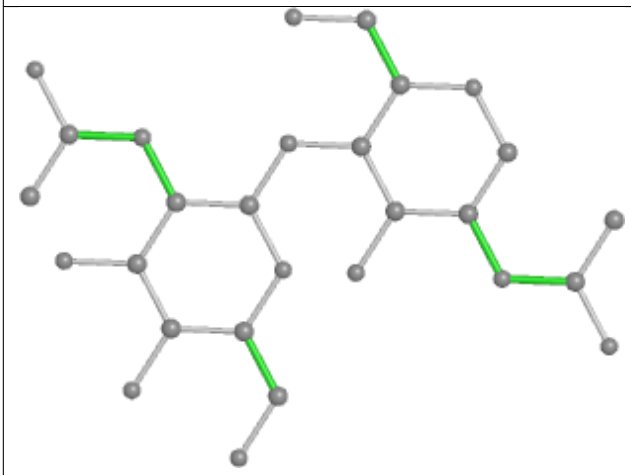


Bond angles



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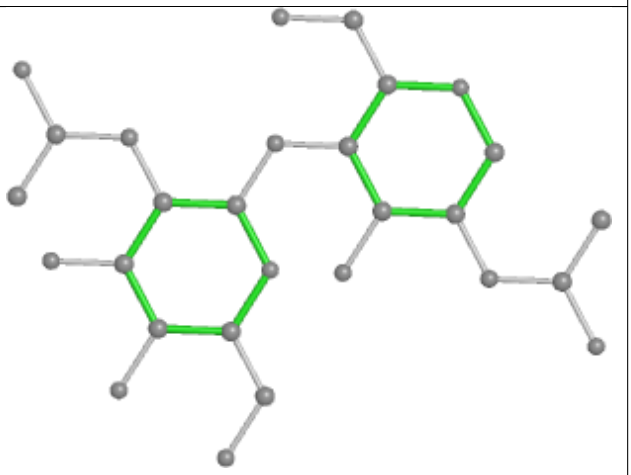
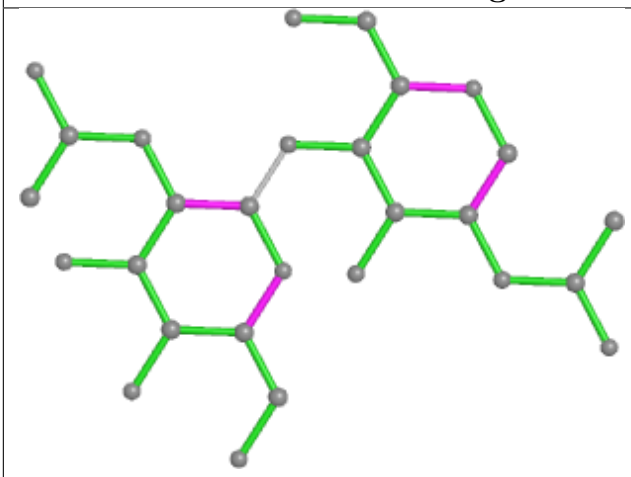


Rings

Oligosaccharide Chain W



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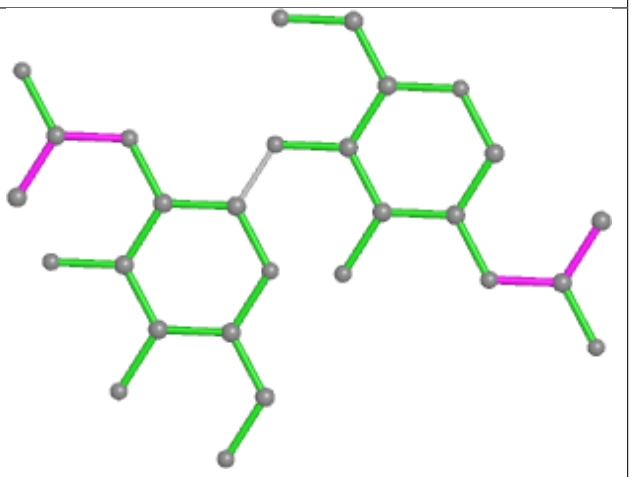

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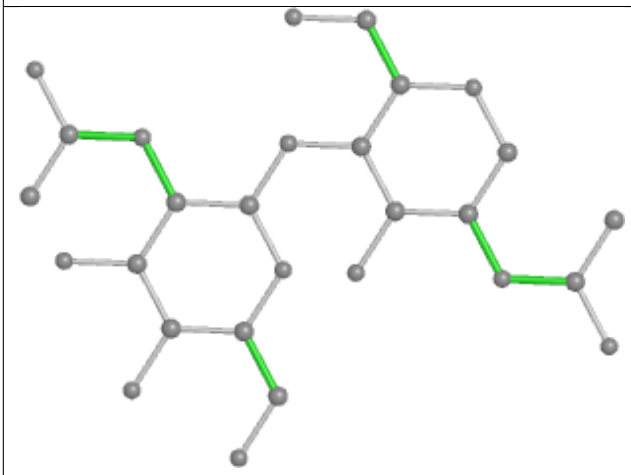
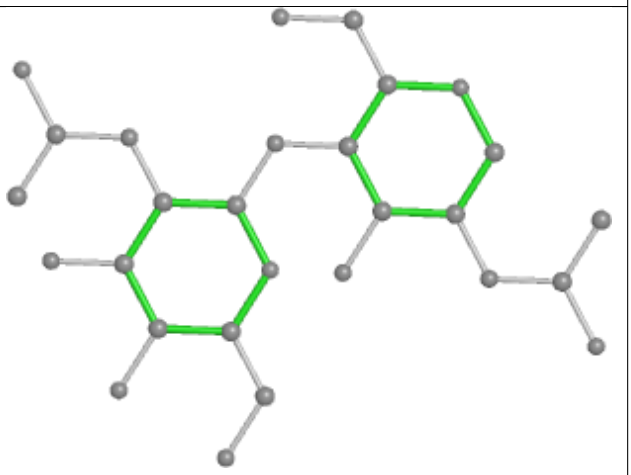
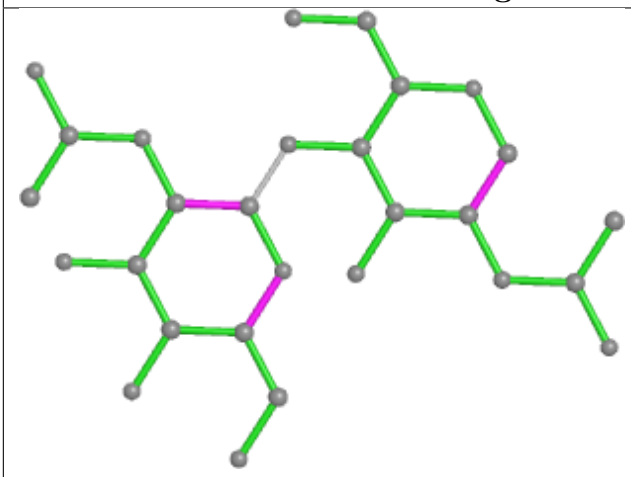


Torsions



Rings

Oligosaccharide Chain X



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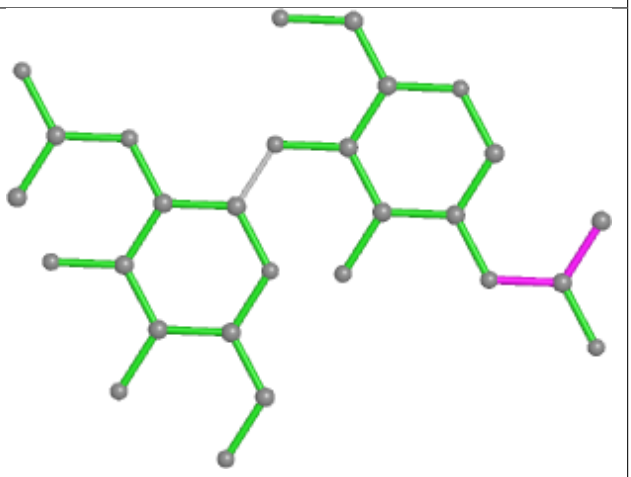
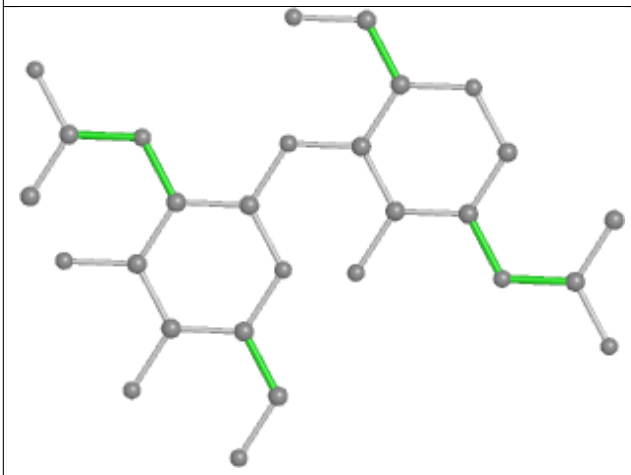
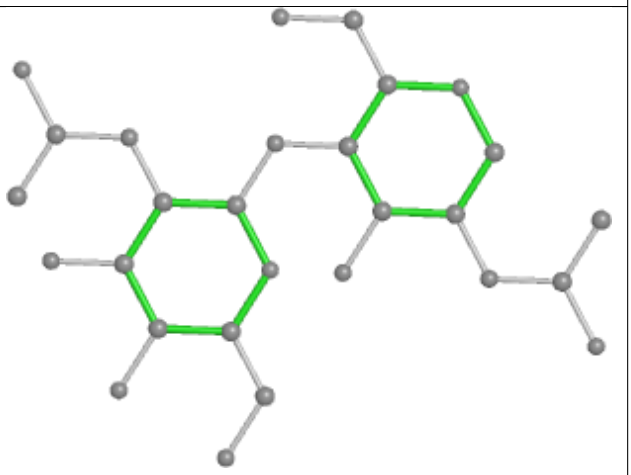


Bond angles

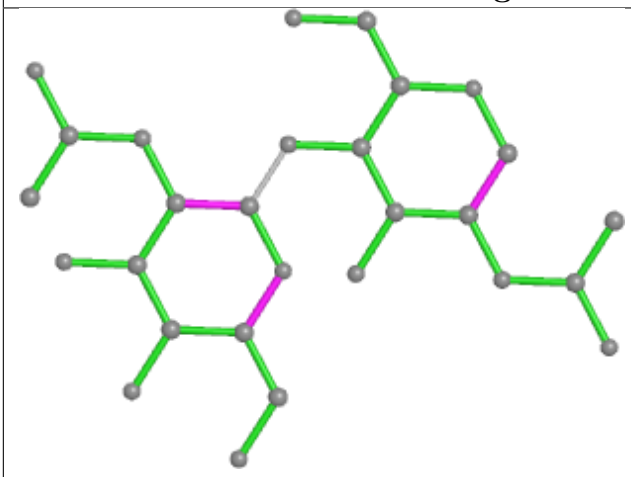


Torsions

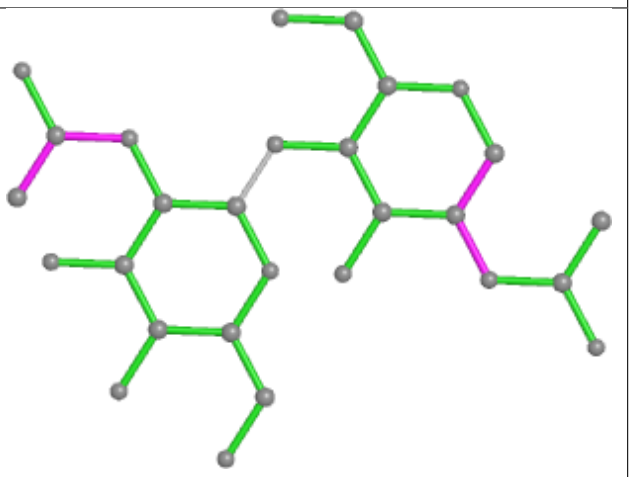


Rings

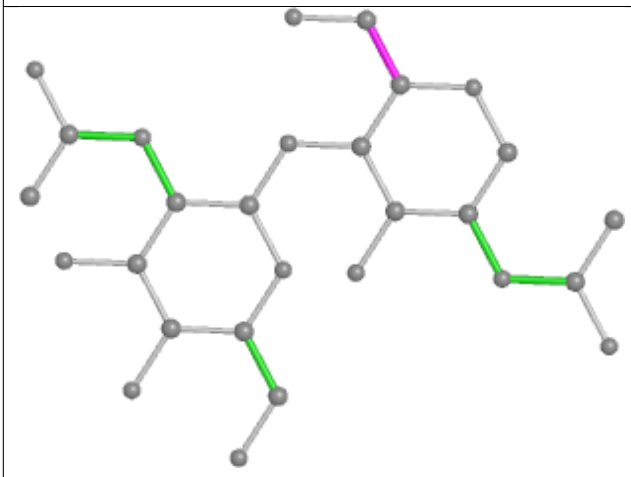
Oligosaccharide Chain Y



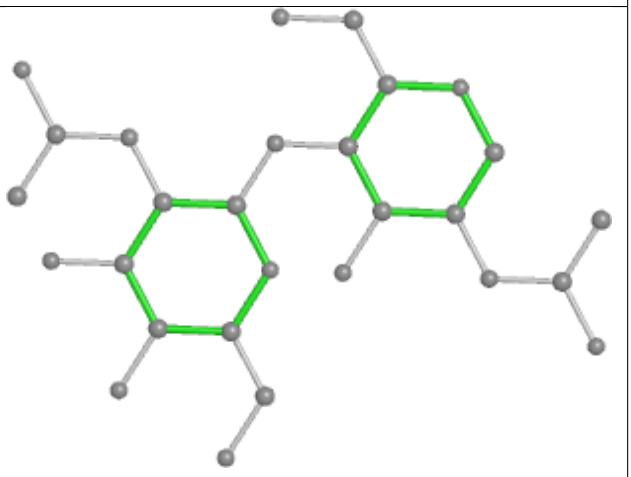
Bond lengths



Bond angles

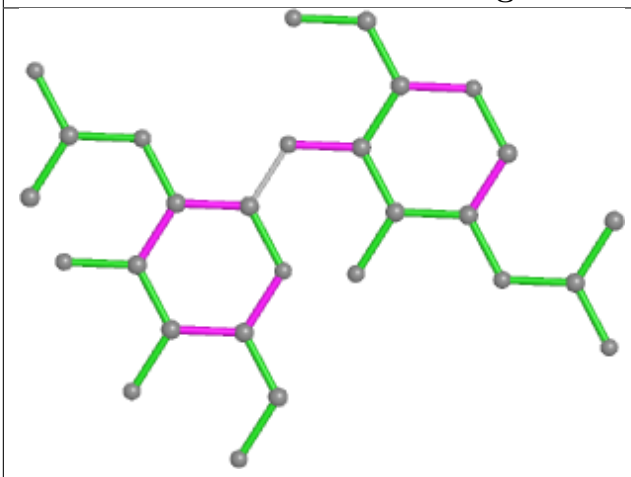


Torsions

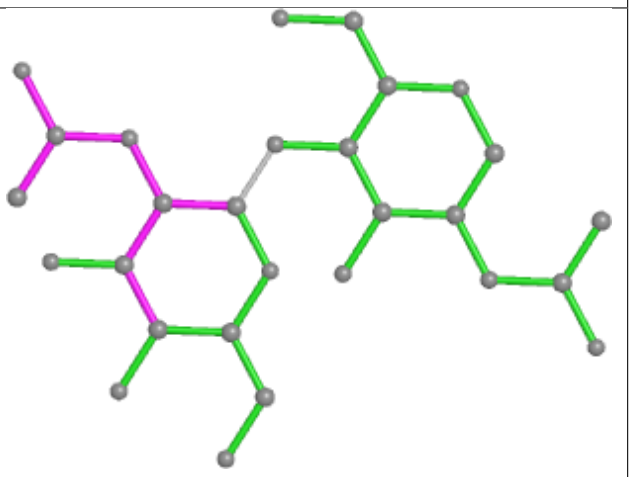


Rings

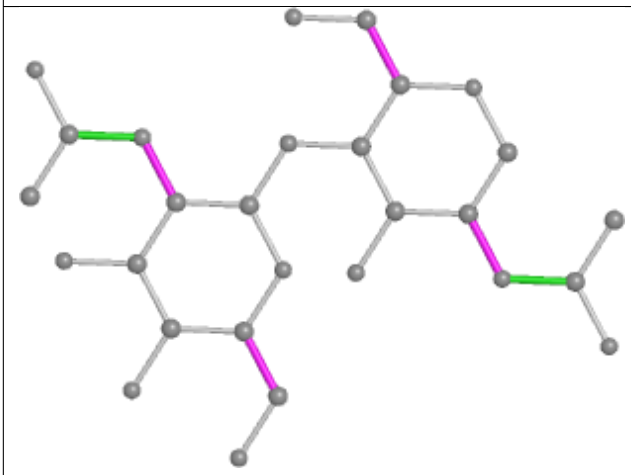
Oligosaccharide Chain Z



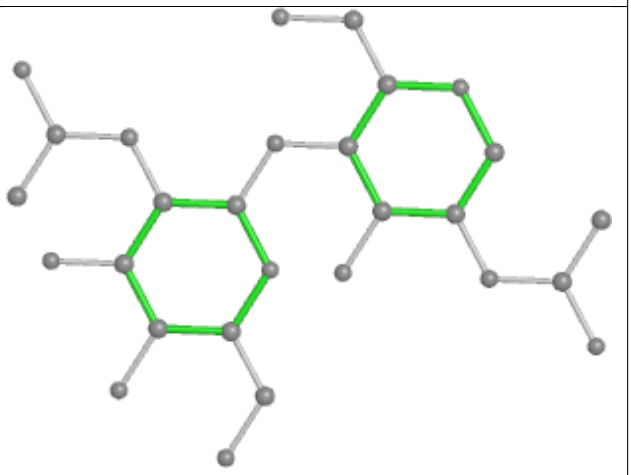
Bond lengths



Bond angles

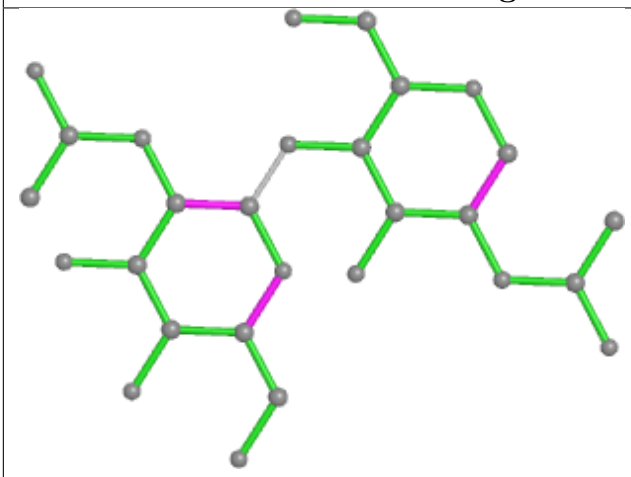


Torsions

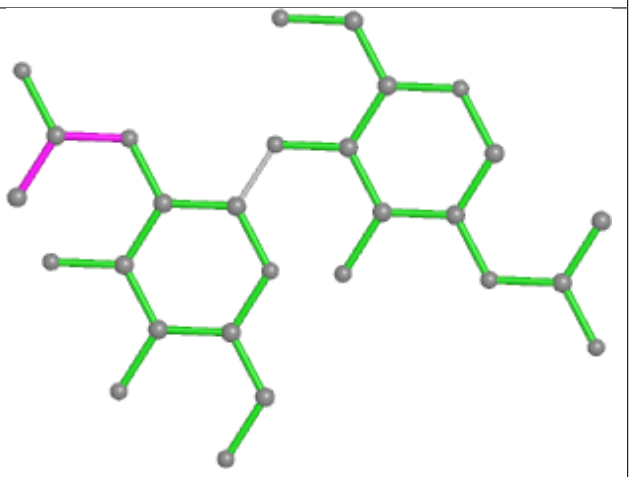


Rings

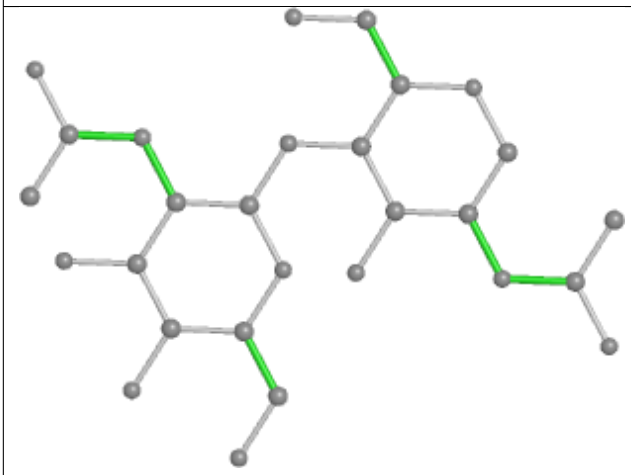
Oligosaccharide Chain a



Bond lengths



Bond angles



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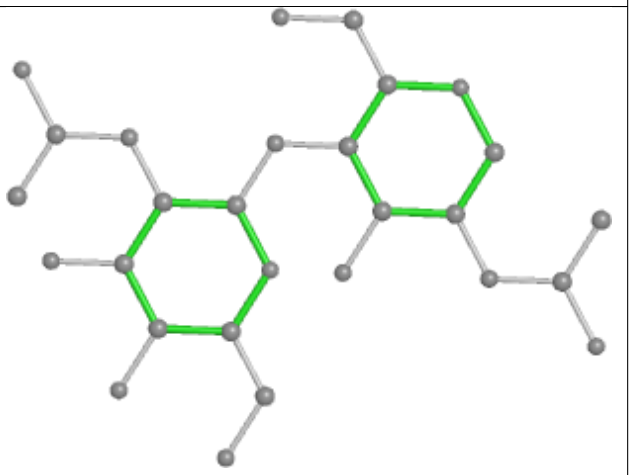
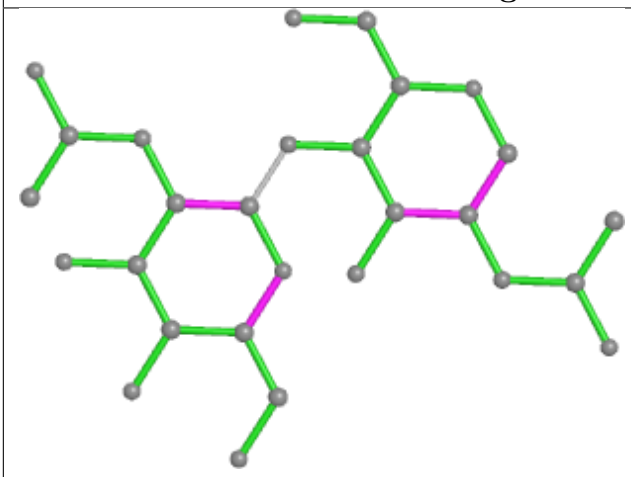
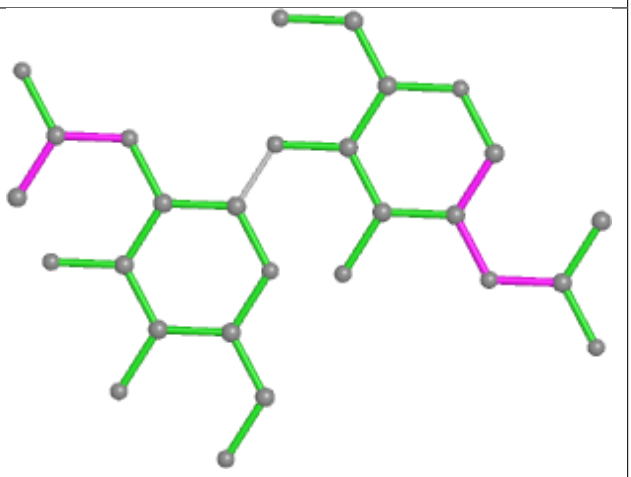


Rings

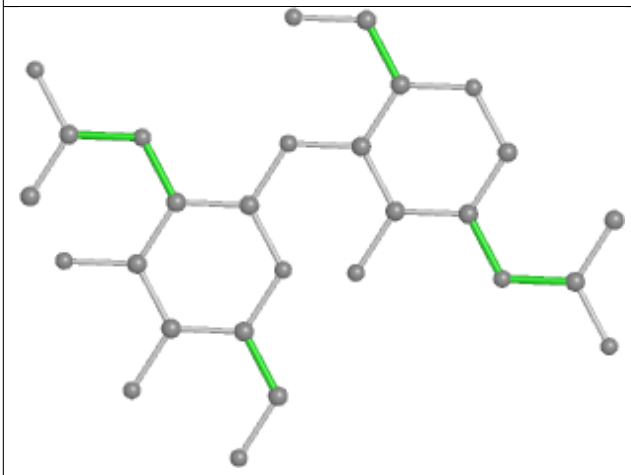
Oligosaccharide Chain c



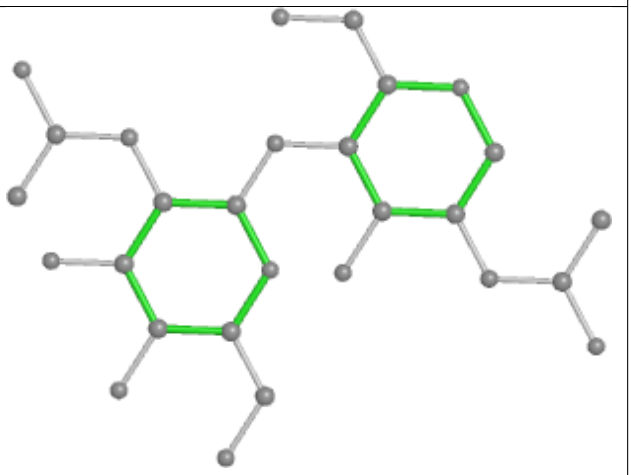
Bond lengths



Bond angles

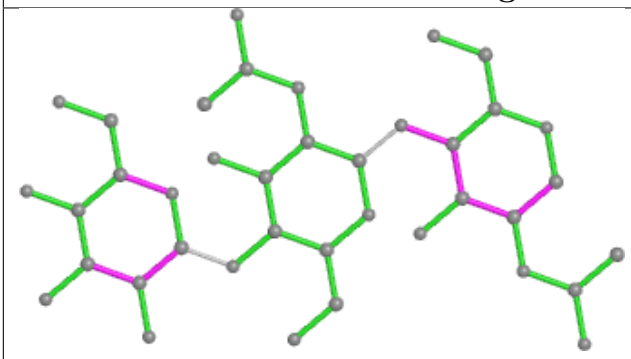


Torsions

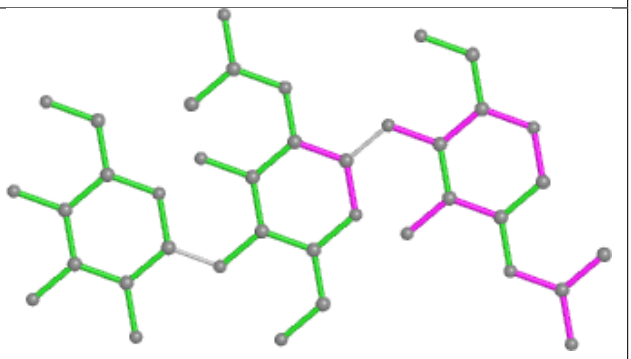


Rings

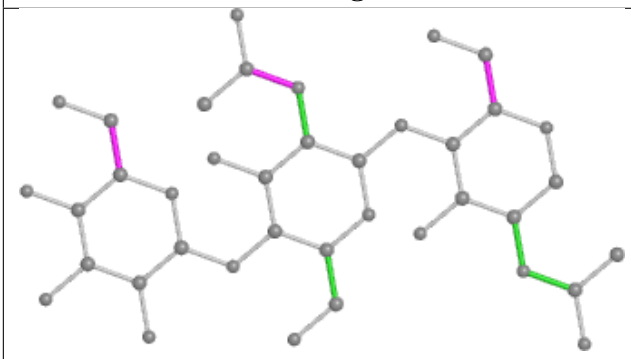
Oligosaccharide Chain J



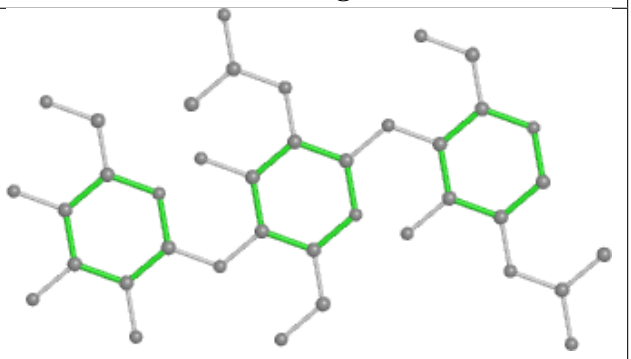
Bond lengths



Bond angles

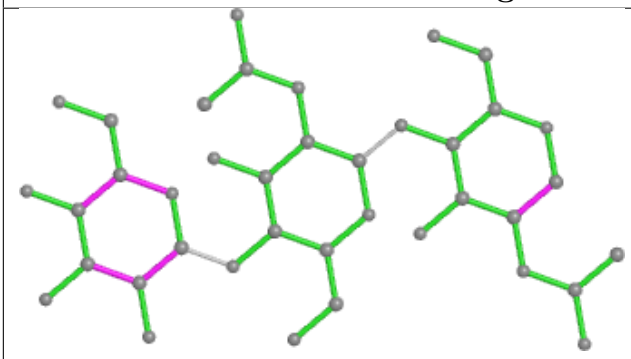


Torsions



Rings

Oligosaccharide Chain L



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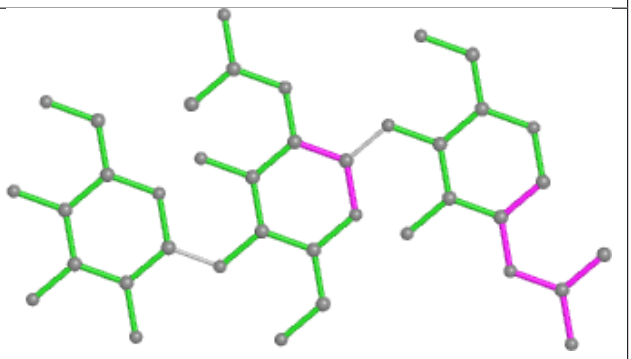
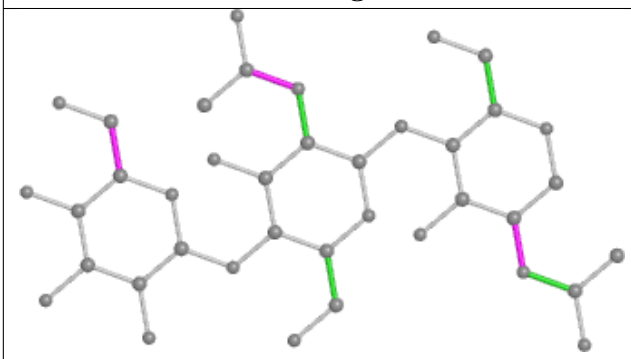


Bond angles



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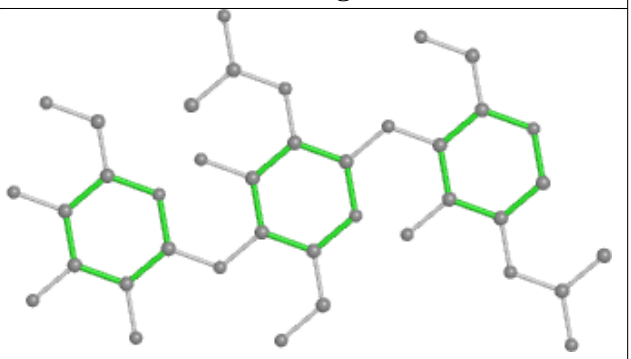
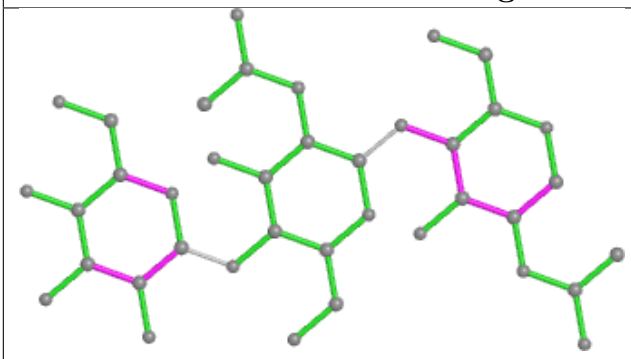


Rings

Oligosaccharide Chain S



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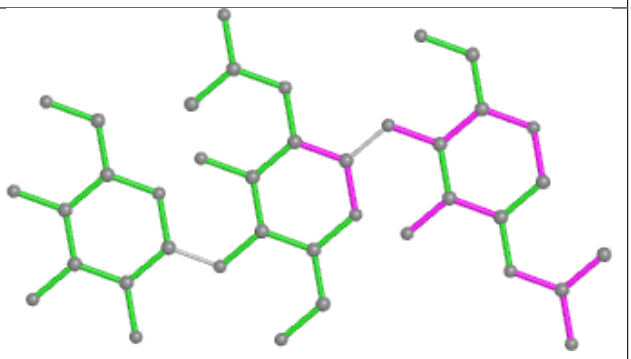
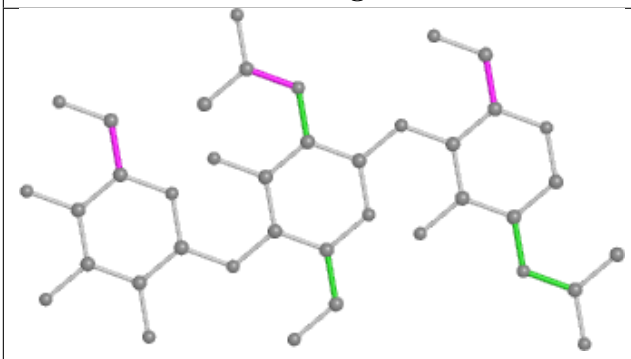
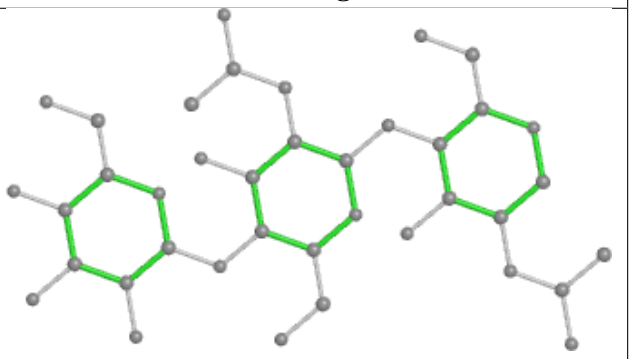


Bond angles

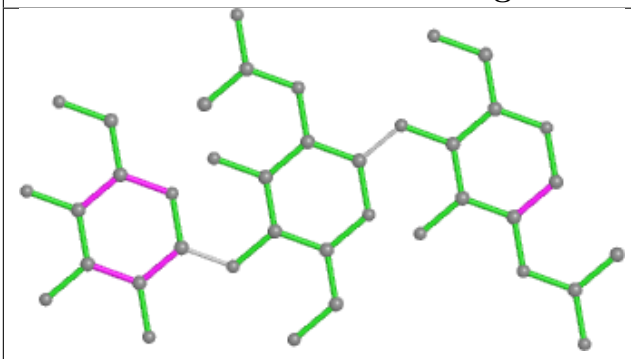


Torsions

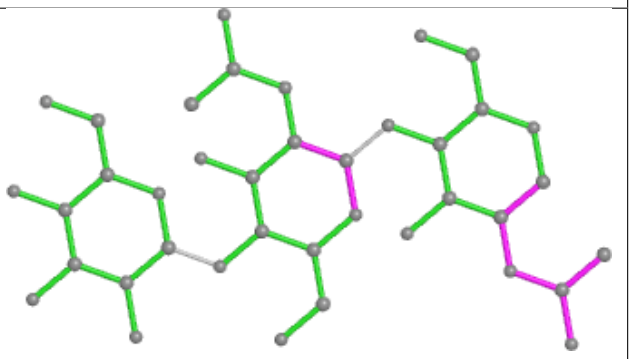


Rings

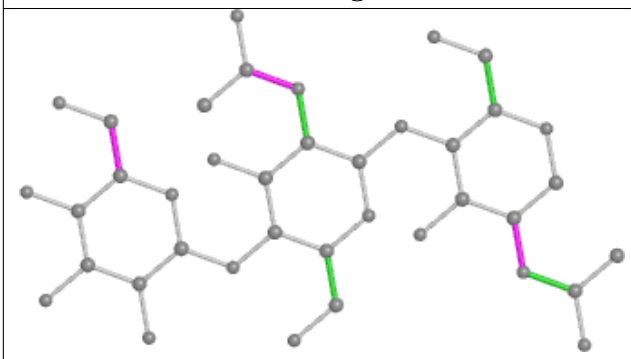
Oligosaccharide Chain U



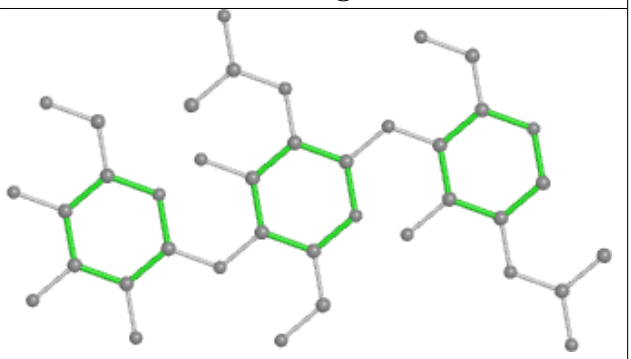
Bond lengths



Bond angles

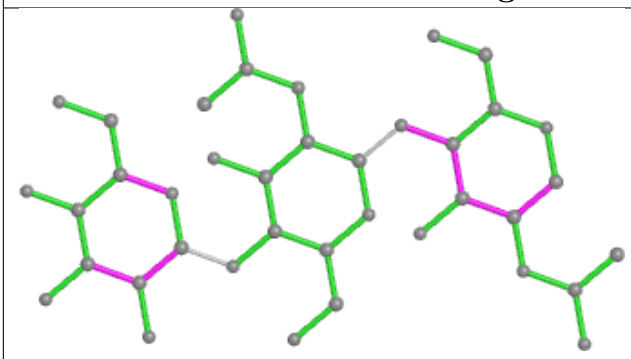


Torsions

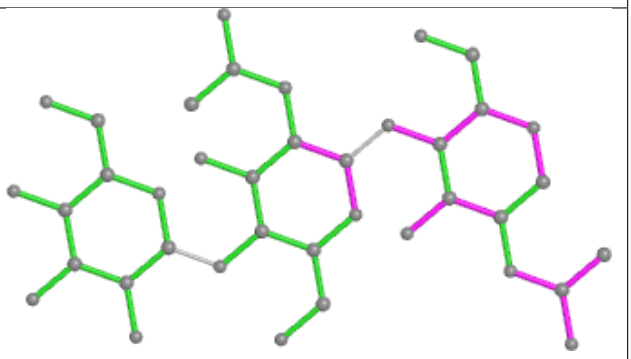


Rings

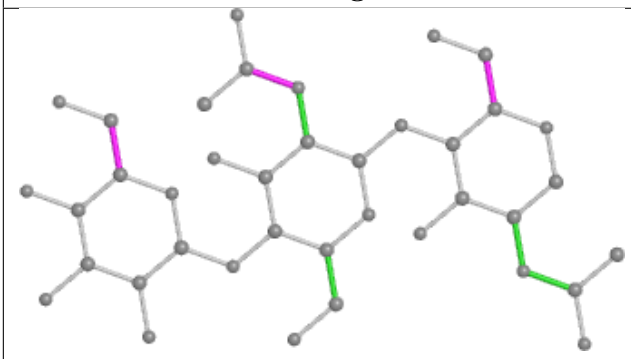
Oligosaccharide Chain b



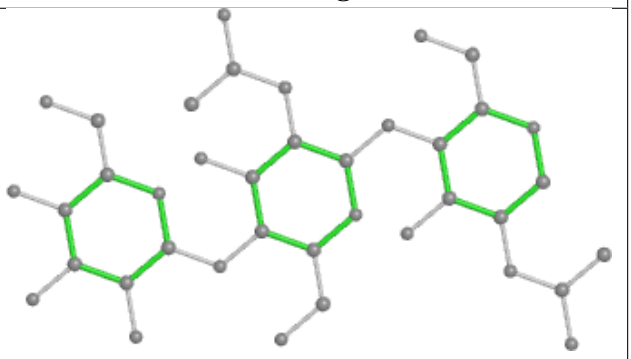
Bond lengths



Bond angles

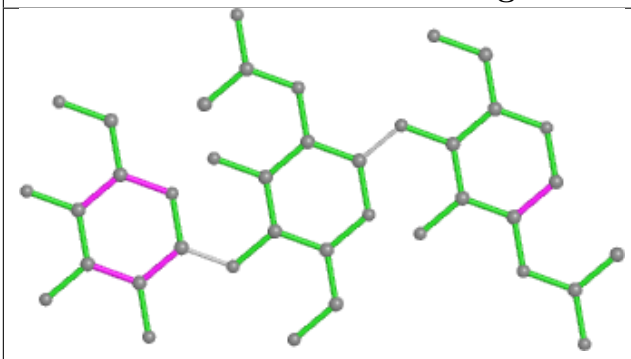


Torsions

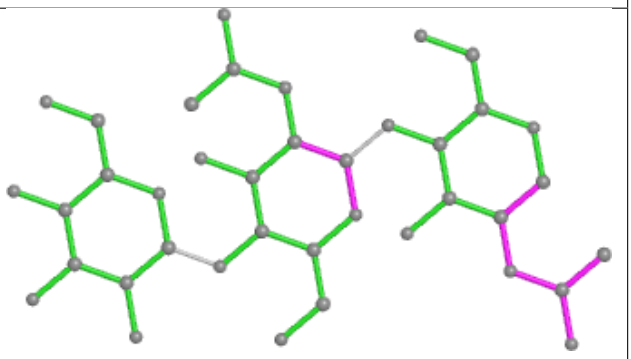


Rings

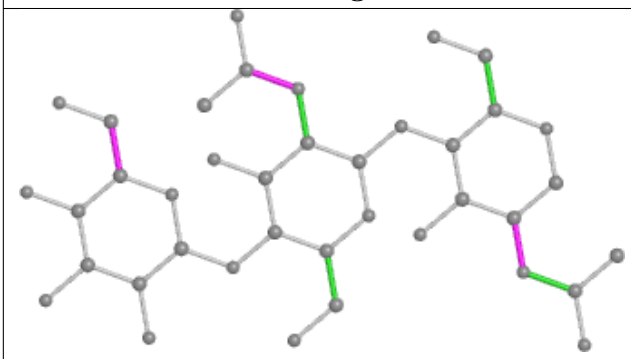
Oligosaccharide Chain d



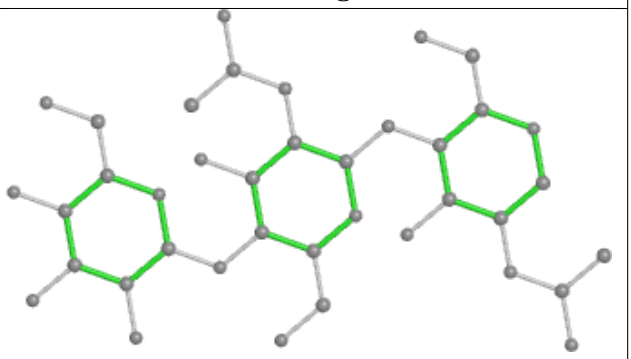
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1508	1	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	A	1501	1	14,14,15	1.49	2 (14%)	17,19,21	1.18	2 (11%)
4	NAG	B	1504	1	14,14,15	1.60	2 (14%)	17,19,21	0.95	1 (5%)
4	NAG	B	1503	1	14,14,15	1.50	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	B	1505	1	14,14,15	1.62	2 (14%)	17,19,21	1.29	2 (11%)
4	NAG	A	1502	1	14,14,15	0.34	0	17,19,21	0.70	0
4	NAG	B	1510	1	14,14,15	0.33	0	17,19,21	0.85	1 (5%)
4	NAG	A	1507	1	14,14,15	1.61	2 (14%)	17,19,21	0.86	1 (5%)
4	NAG	C	1506	1	14,14,15	1.55	2 (14%)	17,19,21	0.90	1 (5%)
4	NAG	A	1510	1	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
4	NAG	C	1501	1	14,14,15	1.48	2 (14%)	17,19,21	1.19	2 (11%)
4	NAG	C	1509	1	14,14,15	1.47	2 (14%)	17,19,21	1.35	1 (5%)
4	NAG	A	1506	1	14,14,15	1.55	2 (14%)	17,19,21	0.90	1 (5%)
4	NAG	A	1505	1	14,14,15	1.61	2 (14%)	17,19,21	1.29	2 (11%)
4	NAG	C	1510	1	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
4	NAG	B	1508	1	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	B	1501	1	14,14,15	1.48	2 (14%)	17,19,21	1.19	2 (11%)
4	NAG	B	1507	1	14,14,15	1.60	2 (14%)	17,19,21	0.86	1 (5%)
4	NAG	C	1507	1	14,14,15	1.60	2 (14%)	17,19,21	0.86	1 (5%)
4	NAG	B	1509	1	14,14,15	1.46	2 (14%)	17,19,21	1.35	1 (5%)
4	NAG	A	1504	1	14,14,15	1.61	2 (14%)	17,19,21	0.96	1 (5%)
4	NAG	C	1505	1	14,14,15	1.61	2 (14%)	17,19,21	1.28	2 (11%)
4	NAG	C	1504	1	14,14,15	1.61	2 (14%)	17,19,21	0.95	1 (5%)
4	NAG	A	1509	1	14,14,15	1.46	2 (14%)	17,19,21	1.35	1 (5%)
4	NAG	A	1503	1	14,14,15	1.50	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	C	1502	1	14,14,15	0.34	0	17,19,21	0.70	0
4	NAG	B	1506	1	14,14,15	1.55	2 (14%)	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1503	1	14,14,15	1.51	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	A	1508	1	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	B	1502	1	14,14,15	0.34	0	17,19,21	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1508	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1504	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1503	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1510	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1507	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1506	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1510	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1509	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1506	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1505	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1510	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1508	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1507	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1507	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1509	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1504	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1505	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1504	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1509	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1503	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1506	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1503	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1508	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	1502	1	-	0/6/23/26	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1504	NAG	C1-C2	4.63	1.59	1.52
4	B	1504	NAG	C1-C2	4.62	1.59	1.52
4	C	1504	NAG	C1-C2	4.62	1.59	1.52
4	B	1505	NAG	C1-C2	4.32	1.58	1.52
4	A	1505	NAG	C1-C2	4.31	1.58	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1509	NAG	C1-C2-N2	-4.88	102.15	110.49
4	A	1509	NAG	C1-C2-N2	-4.88	102.16	110.49
4	B	1509	NAG	C1-C2-N2	-4.87	102.16	110.49
4	B	1505	NAG	C8-C7-N2	3.69	122.35	116.10
4	A	1505	NAG	C8-C7-N2	3.68	122.34	116.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1508	NAG	C1
4	B	1508	NAG	C1
4	C	1508	NAG	C1

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1509	NAG	O5-C5-C6-O6
4	B	1509	NAG	O5-C5-C6-O6
4	C	1509	NAG	O5-C5-C6-O6
4	A	1510	NAG	C8-C7-N2-C2
4	B	1510	NAG	C8-C7-N2-C2

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.

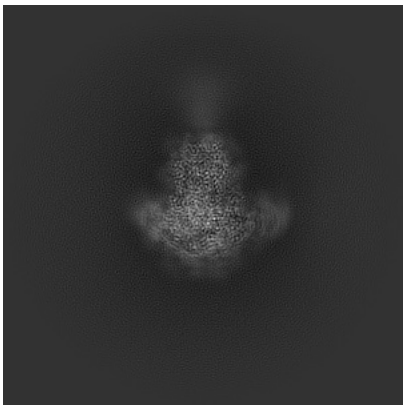
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26730. These allow visual inspection of the internal detail of the map and identification of artifacts.

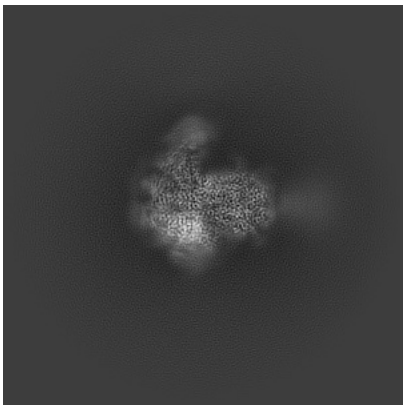
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

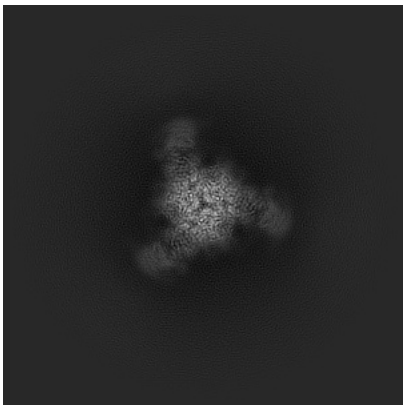
6.1.1 Primary map



X

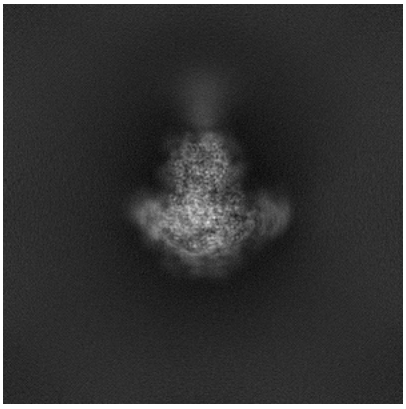


Y

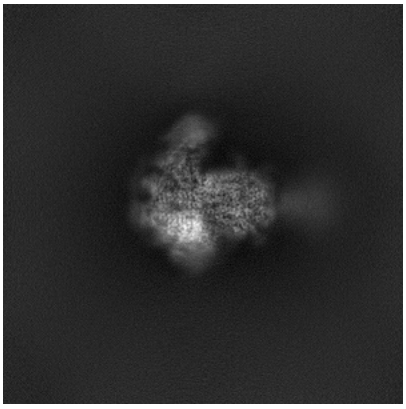


Z

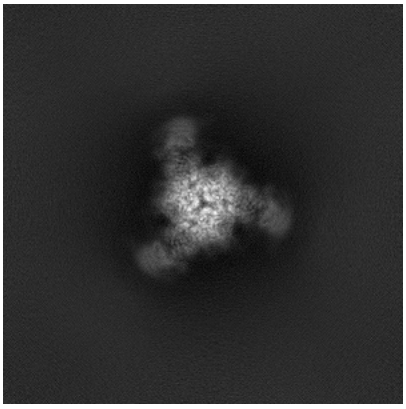
6.1.2 Raw map



X



Y

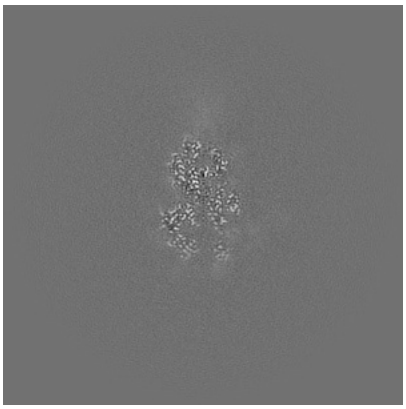


Z

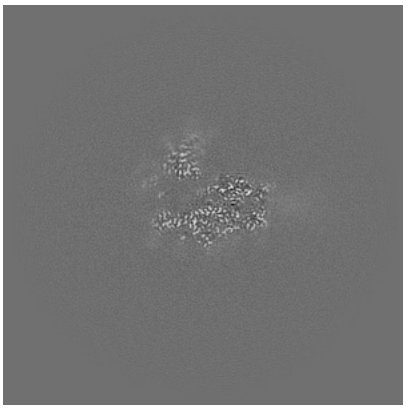
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

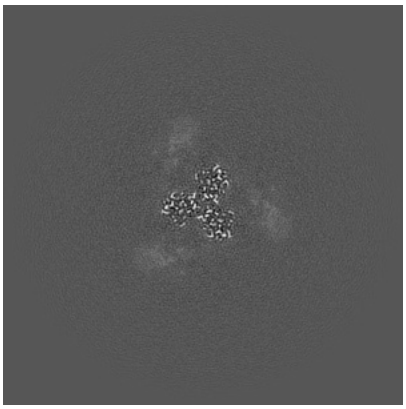
6.2.1 Primary map



X Index: 256

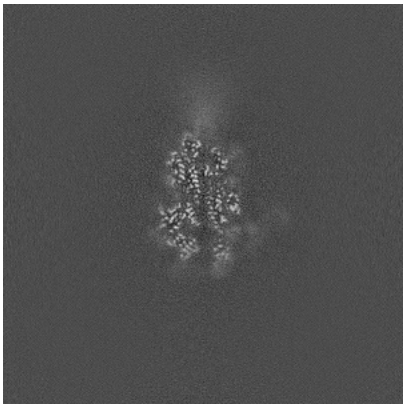


Y Index: 256

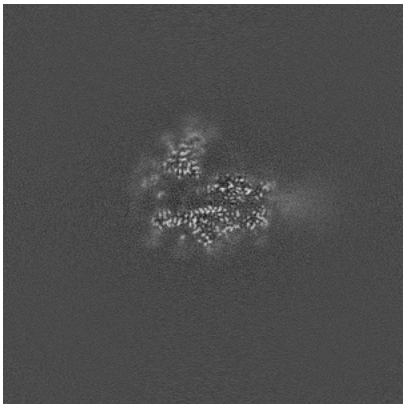


Z Index: 256

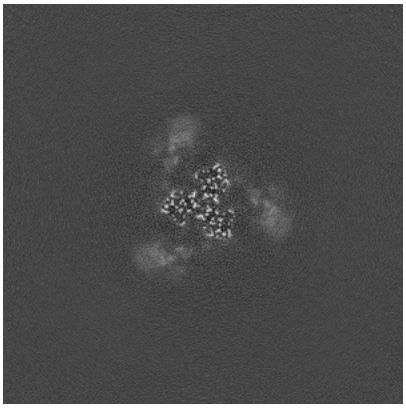
6.2.2 Raw map



X Index: 256



Y Index: 256

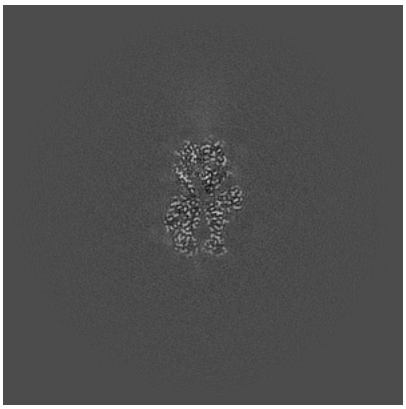


Z Index: 256

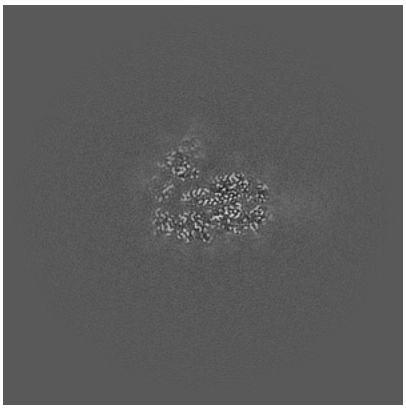
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

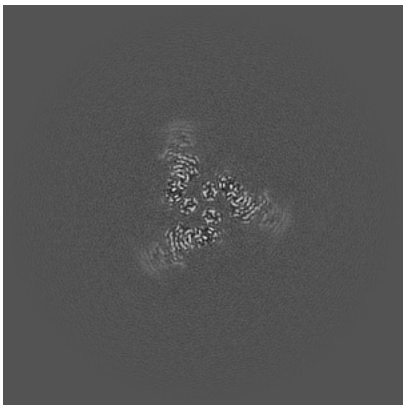
6.3.1 Primary map



X Index: 267

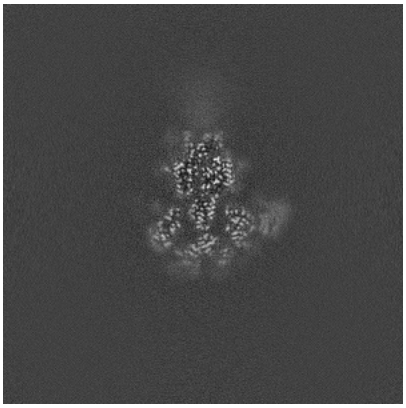


Y Index: 262

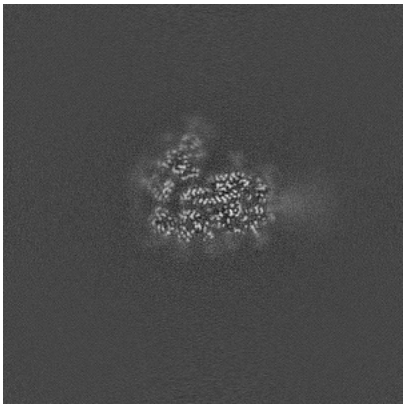


Z Index: 232

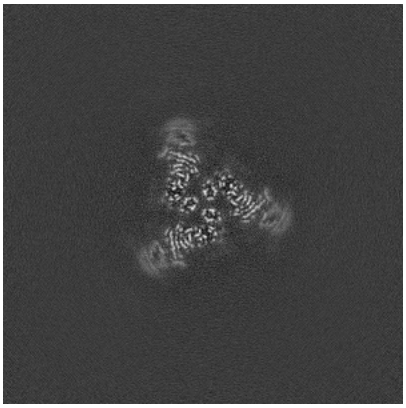
6.3.2 Raw map



X Index: 242



Y Index: 263

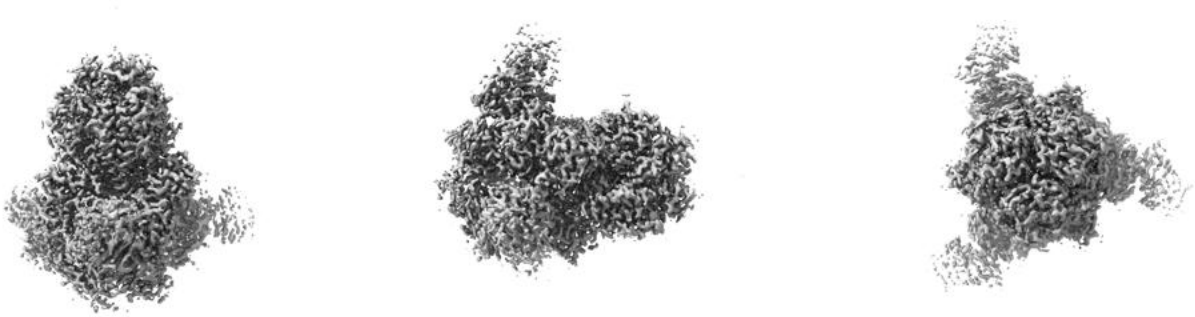


Z Index: 232

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

6.4 Orthogonal surface views (i)

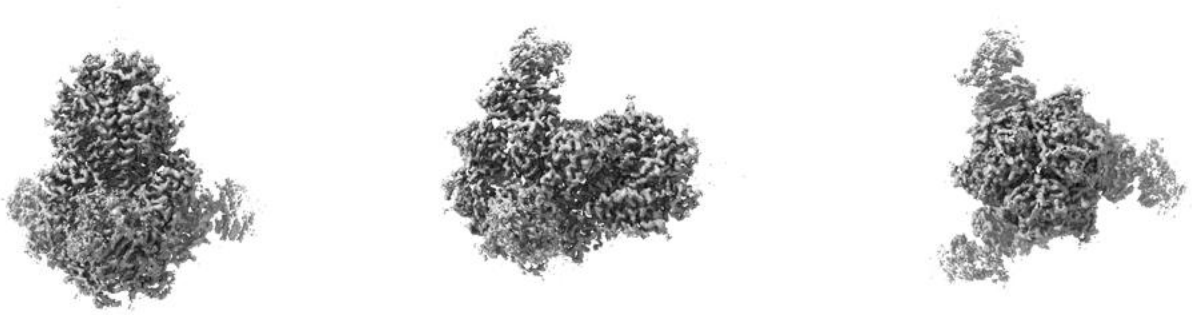
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.706. 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.

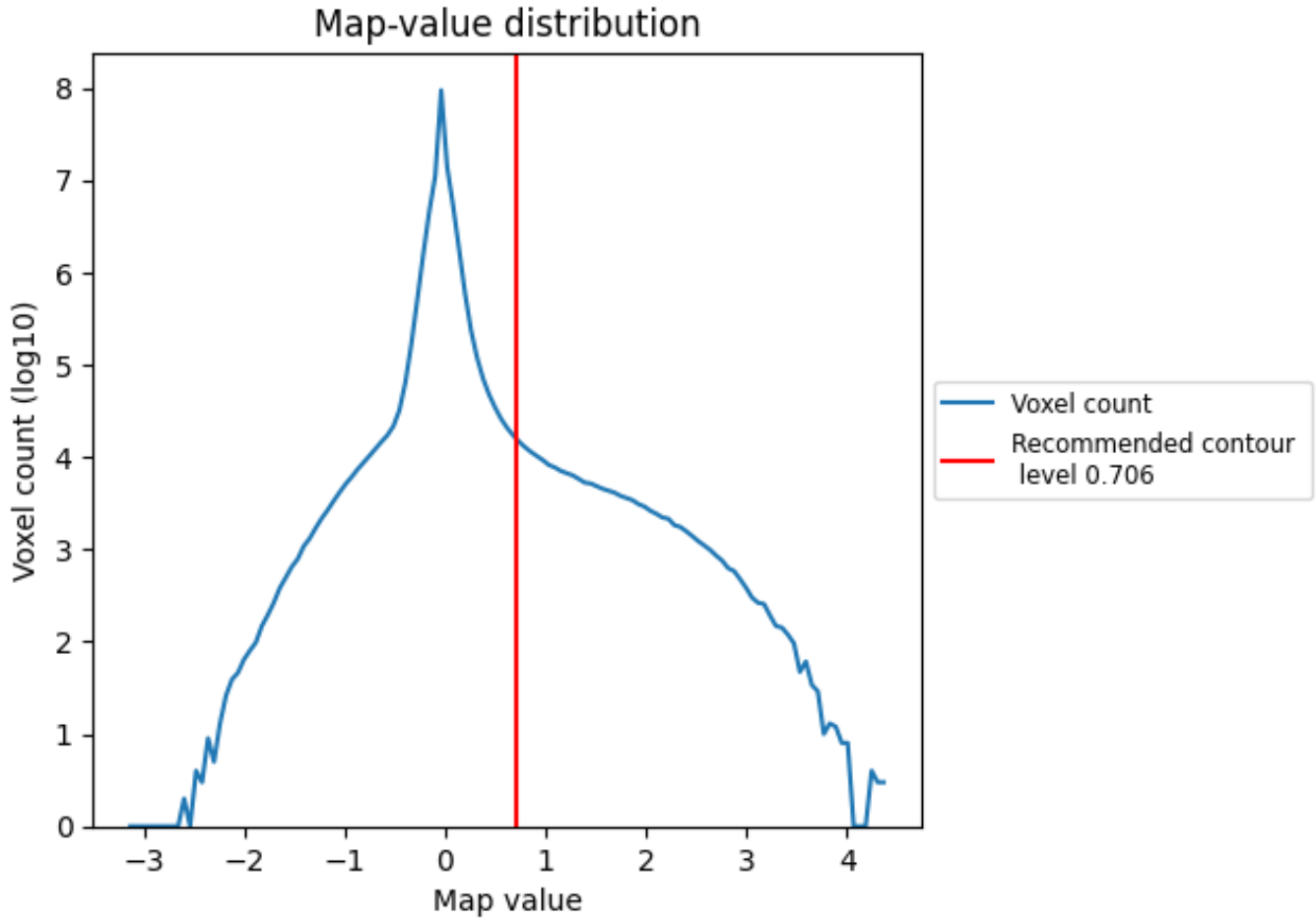
6.5 Mask visualisation (i)

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

7 Map analysis

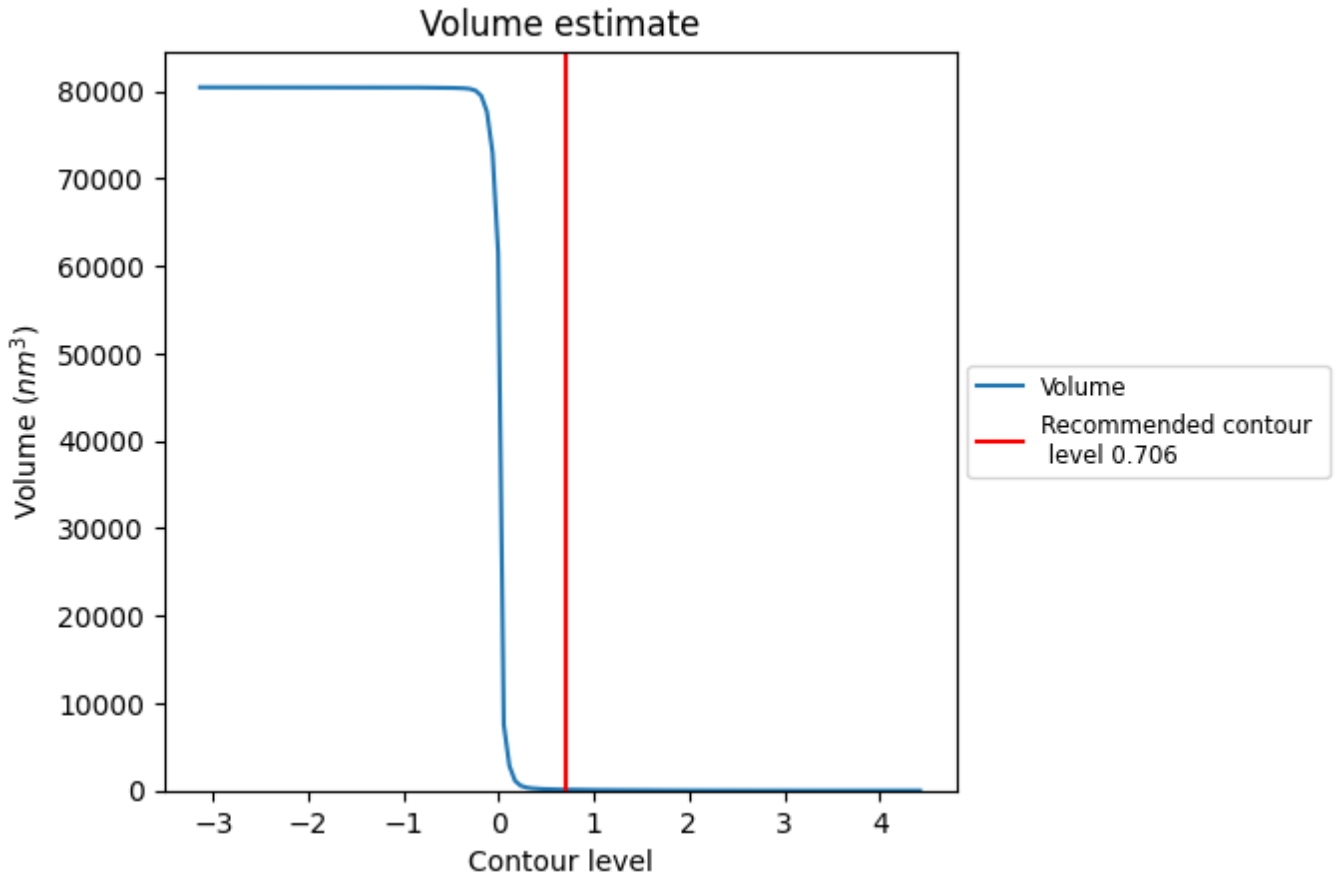
This section contains the results of statistical analysis of the map.

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.

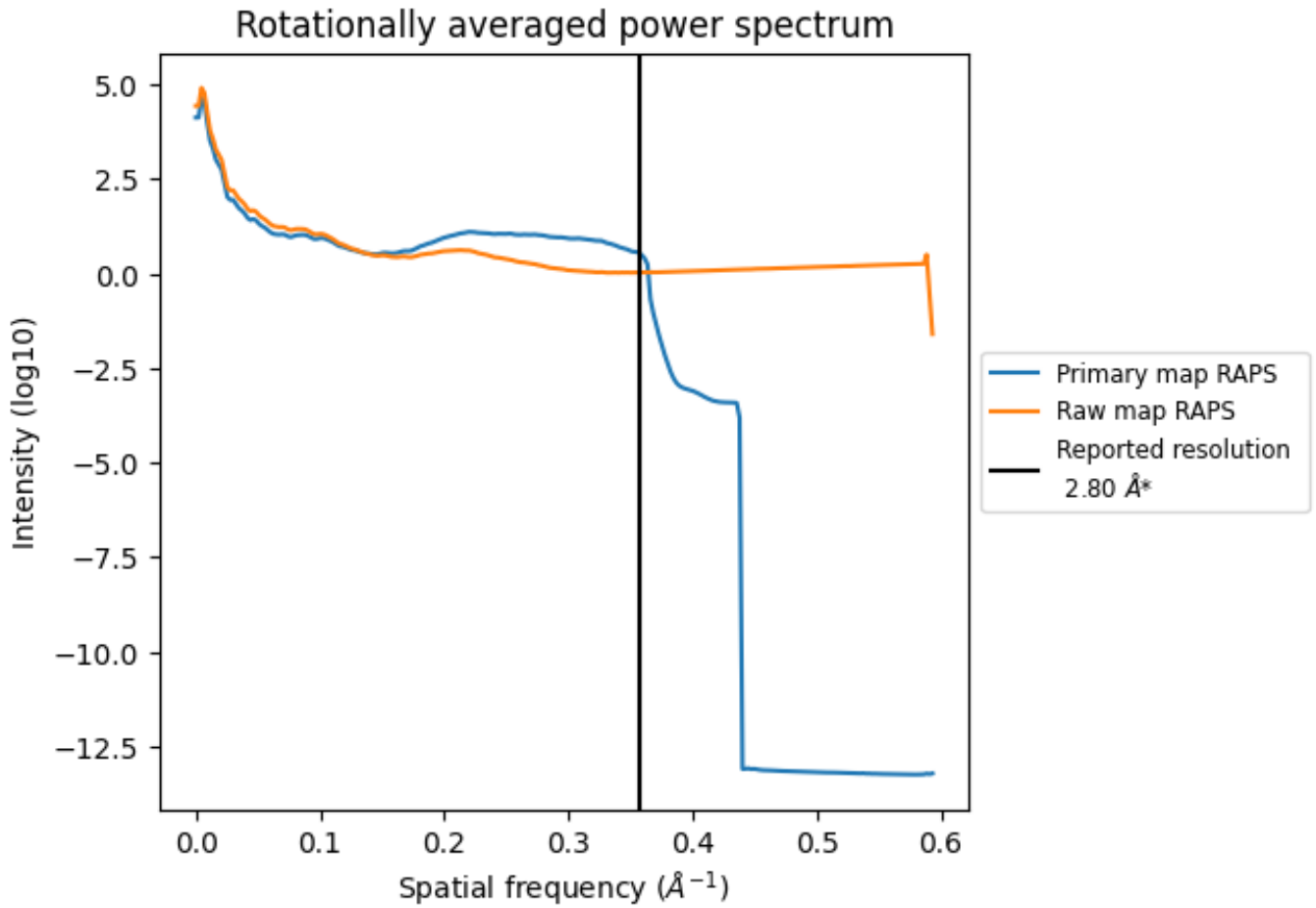
7.2 Volume estimate (i)



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

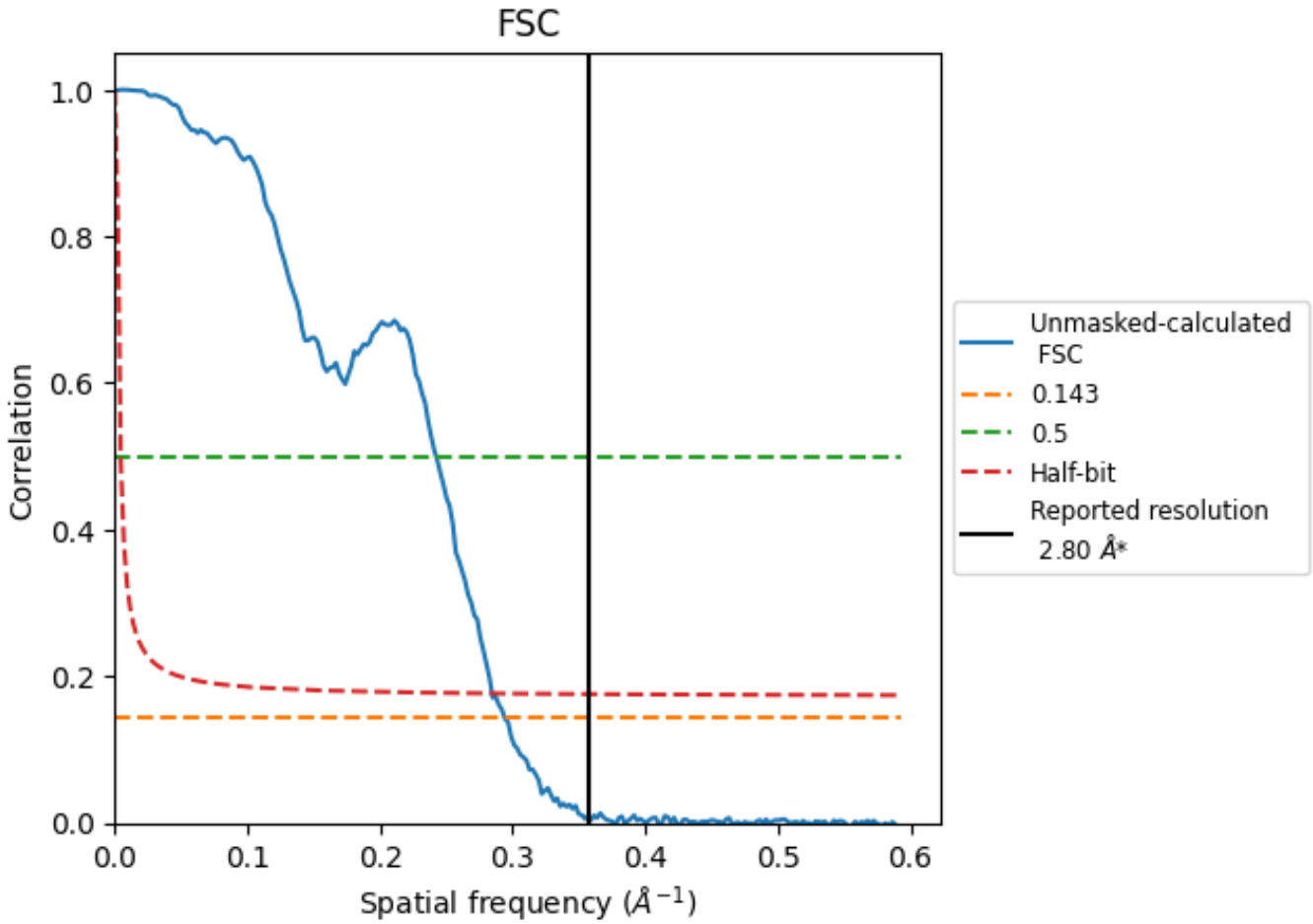


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

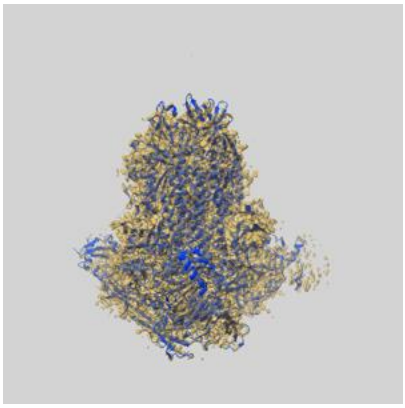
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	4.13	3.52

*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 3.40 differs from the reported value 2.8 by more than 10 %

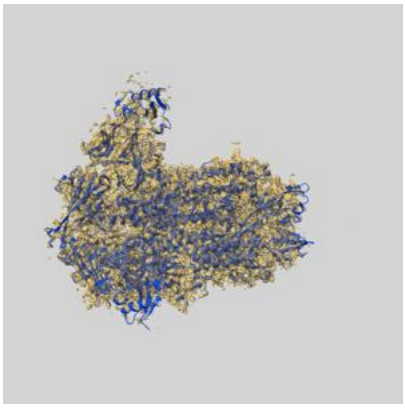
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26730 and PDB model 7USA. Per-residue inclusion information can be found in section 3 on page 17.

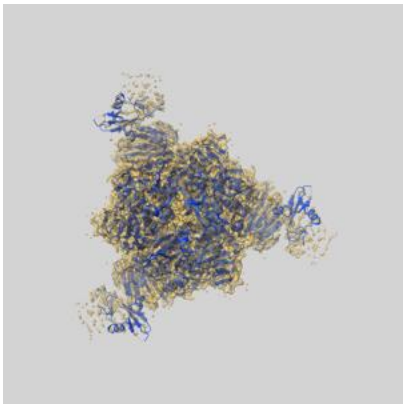
9.1 Map-model overlay



X



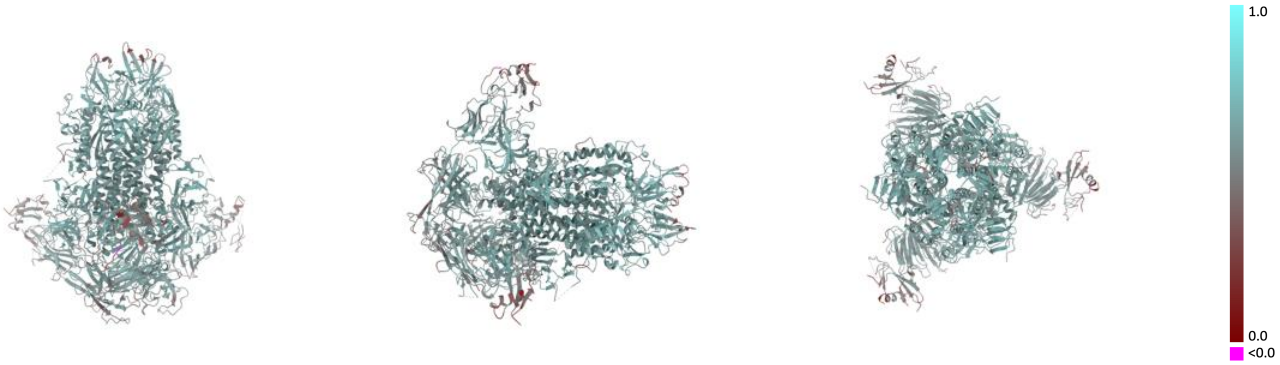
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.706 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.

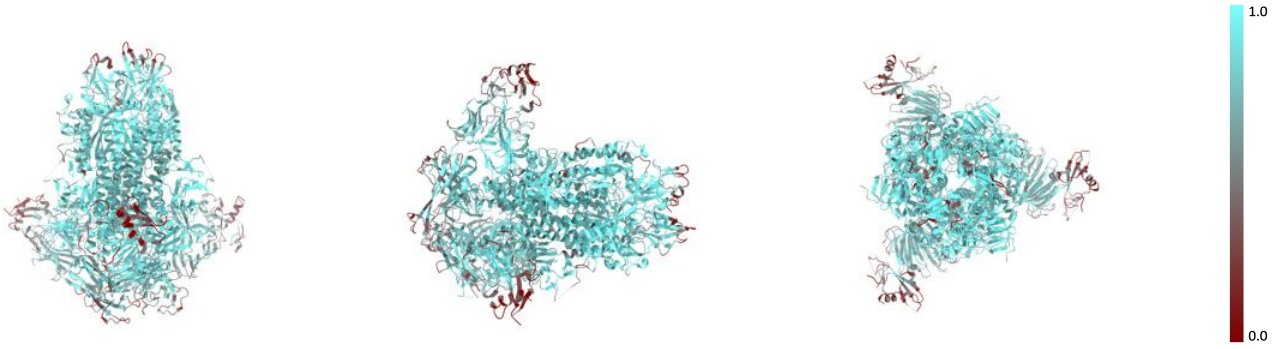
9.2 Q-score mapped to coordinate model (i)



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.

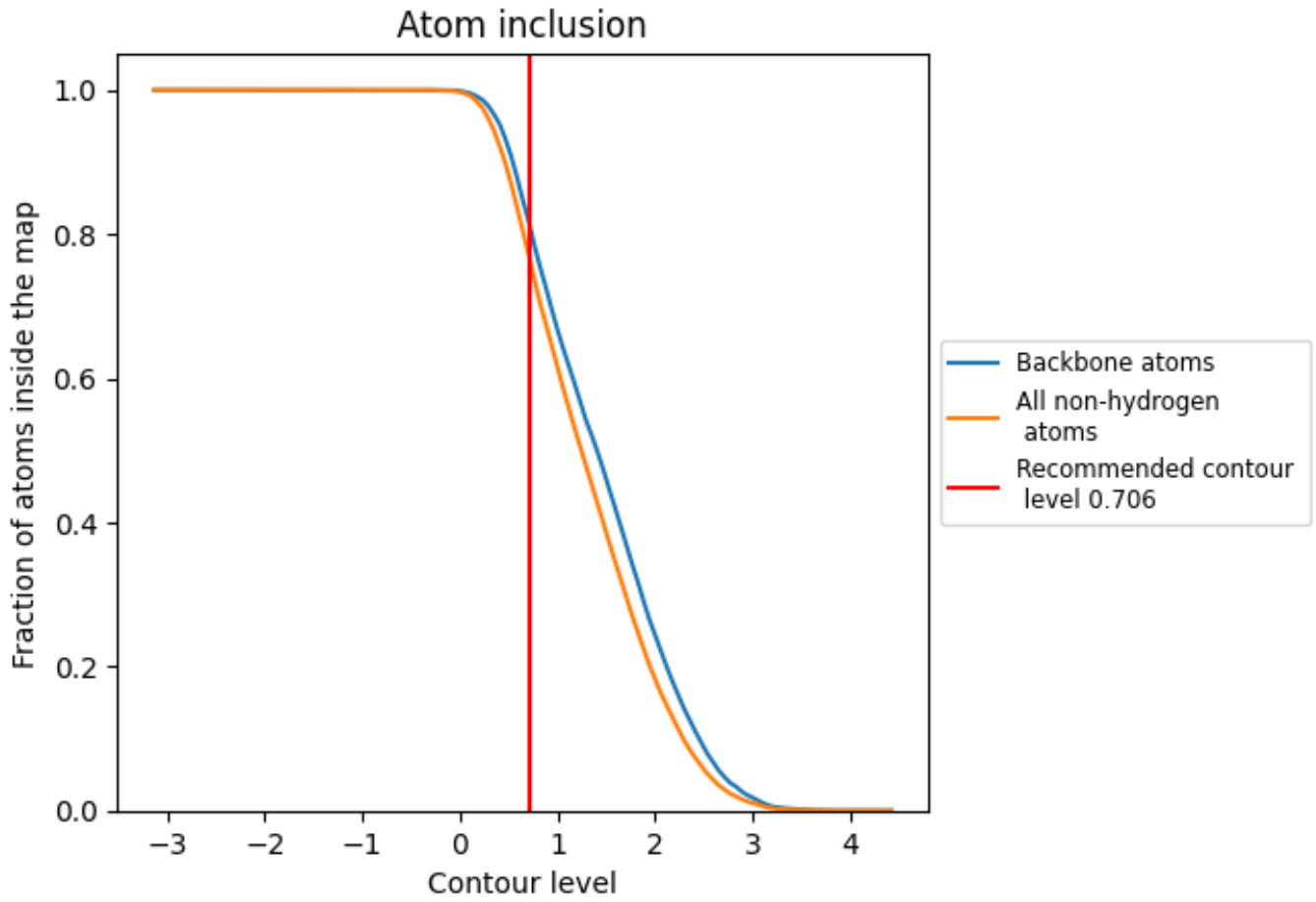
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.706).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.706) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7713	0.5820
A	0.7824	0.5850
B	0.7815	0.5860
C	0.7830	0.5860
D	0.2143	0.4540
E	0.3571	0.4700
F	0.7143	0.5650
G	0.8571	0.5930
H	0.2857	0.3330
I	0.2500	0.4580
J	0.6154	0.5110
K	0.4286	0.4160
L	0.3846	0.4530
M	0.1786	0.4500
N	0.3929	0.4700
O	0.7143	0.5570
P	0.8214	0.5940
Q	0.2857	0.3150
R	0.2857	0.4660
S	0.6410	0.5170
T	0.3929	0.4270
U	0.4103	0.4620
V	0.2143	0.4460
W	0.3571	0.4670
X	0.7143	0.5740
Y	0.8214	0.6030
Z	0.2857	0.3410
a	0.2857	0.4760
b	0.6410	0.5150
c	0.3929	0.4150
d	0.4103	0.4530