Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 03:37 PM EDT

PDB ID	:	7M5E
EMDB ID	:	EMD-23674
Title	:	MERS-CoV S bound to the broadly neutralizing B6 Fab fragment (C3 refinement)
Authors	:	Sauer, M.M.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2021-03-23
Resolution	:	2.50 Å(reported)

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

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

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

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

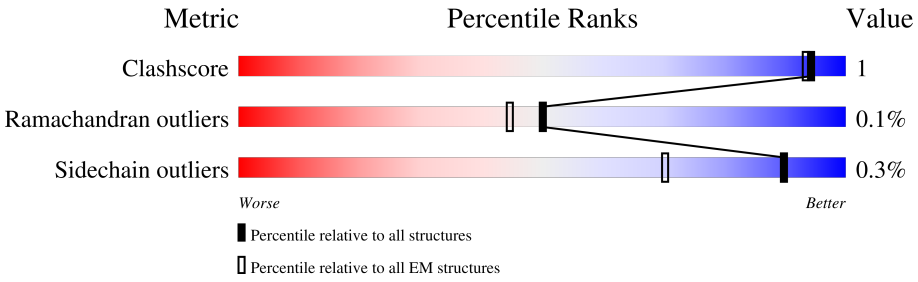
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1359	82% · 15%
1	C	1359	82% · 15%
1	E	1359	82% · 15%
2	B	4	25% 100%
2	H	4	50% 100%
2	N	4	25% 100%
2	R	4	50% 100%
2	X	4	25% 100%

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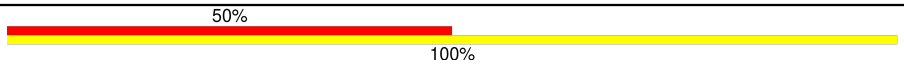
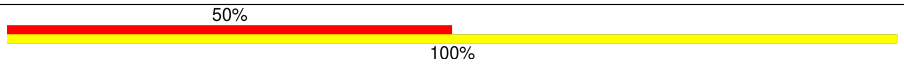
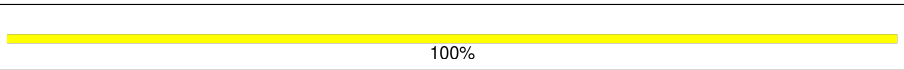
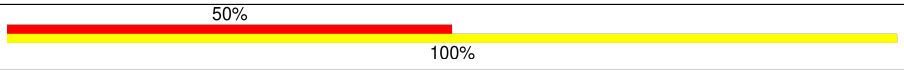
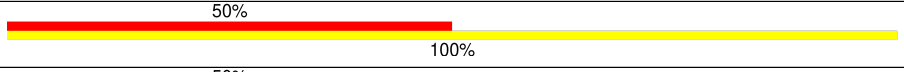
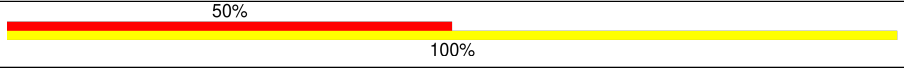
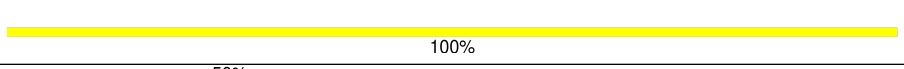
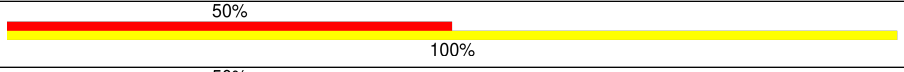
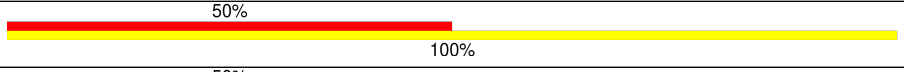
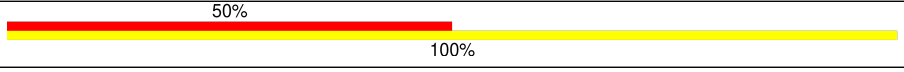
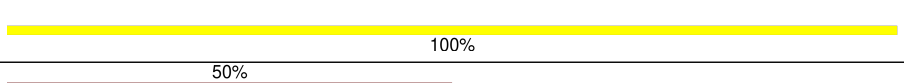
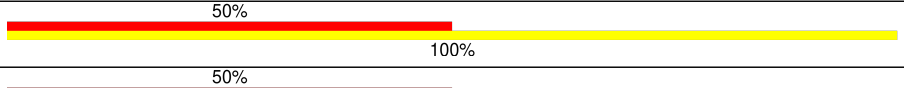
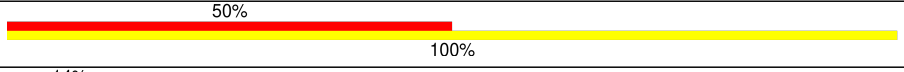
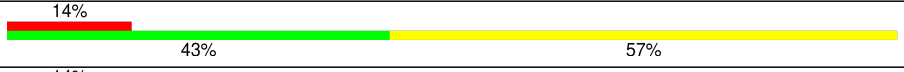
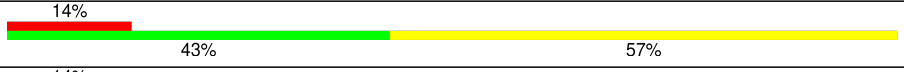
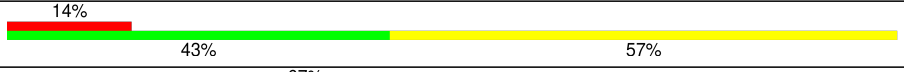
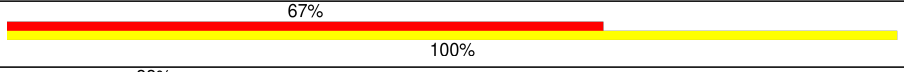
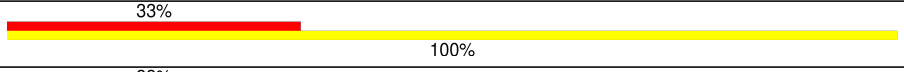
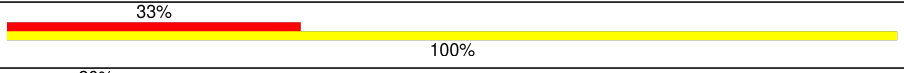
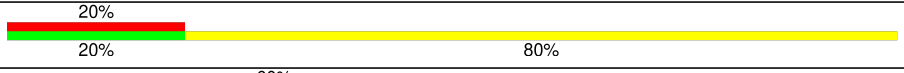
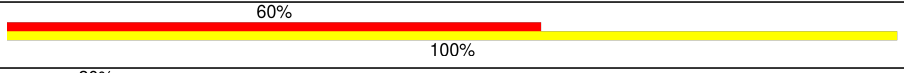
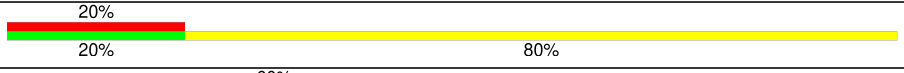
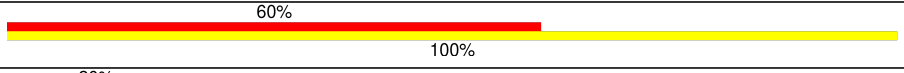
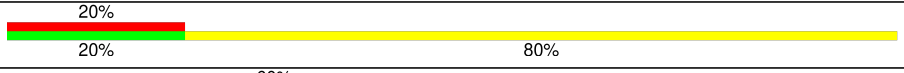
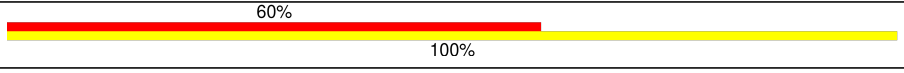
Mol	Chain	Length	Quality of chain
2	b	4	
3	D	2	
3	I	2	
3	J	2	
3	M	2	
3	O	2	
3	S	2	
3	T	2	
3	W	2	
3	Y	2	
3	c	2	
3	d	2	
3	g	2	
4	F	7	
4	P	7	
4	Z	7	
5	G	3	
5	Q	3	
5	a	3	
6	K	5	
6	L	5	
6	U	5	
6	V	5	
6	e	5	
6	f	5	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 28566 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	1159	Total	C	N	O	S	0	0
			8915	5674	1472	1720	49		
1	C	1159	Total	C	N	O	S	0	0
			8915	5674	1472	1720	49		
1	E	1159	Total	C	N	O	S	0	0
			8915	5674	1472	1720	49		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A140AYW5
A	-12	GLY	-	expression tag	UNP A0A140AYW5
A	-11	ILE	-	expression tag	UNP A0A140AYW5
A	-10	LEU	-	expression tag	UNP A0A140AYW5
A	-9	PRO	-	expression tag	UNP A0A140AYW5
A	-8	SER	-	expression tag	UNP A0A140AYW5
A	-7	PRO	-	expression tag	UNP A0A140AYW5
A	-6	GLY	-	expression tag	UNP A0A140AYW5
A	-5	MET	-	expression tag	UNP A0A140AYW5
A	-4	PRO	-	expression tag	UNP A0A140AYW5
A	-3	ALA	-	expression tag	UNP A0A140AYW5
A	-2	LEU	-	expression tag	UNP A0A140AYW5
A	-1	LEU	-	expression tag	UNP A0A140AYW5
A	0	SER	-	expression tag	UNP A0A140AYW5
A	1	LEU	-	expression tag	UNP A0A140AYW5
A	2	VAL	-	expression tag	UNP A0A140AYW5
A	3	SER	-	expression tag	UNP A0A140AYW5
A	4	LEU	-	expression tag	UNP A0A140AYW5
A	5	LEU	-	expression tag	UNP A0A140AYW5
A	6	SER	-	expression tag	UNP A0A140AYW5
A	7	VAL	-	expression tag	UNP A0A140AYW5
A	8	LEU	-	expression tag	UNP A0A140AYW5
A	9	LEU	-	expression tag	UNP A0A140AYW5
A	10	MET	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP A0A140AYW5
A	12	CYS	-	expression tag	UNP A0A140AYW5
A	13	VAL	-	expression tag	UNP A0A140AYW5
A	14	ALA	-	expression tag	UNP A0A140AYW5
A	15	GLU	-	expression tag	UNP A0A140AYW5
A	16	THR	-	expression tag	UNP A0A140AYW5
A	17	GLY	-	expression tag	UNP A0A140AYW5
A	18	THR	-	expression tag	UNP A0A140AYW5
A	529	ILE	THR	conflict	UNP A0A140AYW5
A	748	ALA	ARG	conflict	UNP A0A140AYW5
A	751	GLY	ARG	conflict	UNP A0A140AYW5
A	1020	GLN	ARG	conflict	UNP A0A140AYW5
A	1060	PRO	VAL	conflict	UNP A0A140AYW5
A	1061	PRO	LEU	conflict	UNP A0A140AYW5
A	1295	GLY	-	expression tag	UNP A0A140AYW5
A	1296	SER	-	expression tag	UNP A0A140AYW5
A	1297	GLY	-	expression tag	UNP A0A140AYW5
A	1298	ARG	-	expression tag	UNP A0A140AYW5
A	1299	GLU	-	expression tag	UNP A0A140AYW5
A	1300	ASN	-	expression tag	UNP A0A140AYW5
A	1301	LEU	-	expression tag	UNP A0A140AYW5
A	1302	TYR	-	expression tag	UNP A0A140AYW5
A	1303	PHE	-	expression tag	UNP A0A140AYW5
A	1304	GLN	-	expression tag	UNP A0A140AYW5
A	1305	GLY	-	expression tag	UNP A0A140AYW5
A	1306	GLY	-	expression tag	UNP A0A140AYW5
A	1307	GLY	-	expression tag	UNP A0A140AYW5
A	1308	GLY	-	expression tag	UNP A0A140AYW5
A	1309	SER	-	expression tag	UNP A0A140AYW5
A	1310	GLY	-	expression tag	UNP A0A140AYW5
A	1311	TYR	-	expression tag	UNP A0A140AYW5
A	1312	ILE	-	expression tag	UNP A0A140AYW5
A	1313	PRO	-	expression tag	UNP A0A140AYW5
A	1314	GLU	-	expression tag	UNP A0A140AYW5
A	1315	ALA	-	expression tag	UNP A0A140AYW5
A	1316	PRO	-	expression tag	UNP A0A140AYW5
A	1317	ARG	-	expression tag	UNP A0A140AYW5
A	1318	ASP	-	expression tag	UNP A0A140AYW5
A	1319	GLY	-	expression tag	UNP A0A140AYW5
A	1320	GLN	-	expression tag	UNP A0A140AYW5
A	1321	ALA	-	expression tag	UNP A0A140AYW5
A	1322	TYR	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1323	VAL	-	expression tag	UNP A0A140AYW5
A	1324	ARG	-	expression tag	UNP A0A140AYW5
A	1325	LYS	-	expression tag	UNP A0A140AYW5
A	1326	ASP	-	expression tag	UNP A0A140AYW5
A	1327	GLY	-	expression tag	UNP A0A140AYW5
A	1328	GLU	-	expression tag	UNP A0A140AYW5
A	1329	TRP	-	expression tag	UNP A0A140AYW5
A	1330	VAL	-	expression tag	UNP A0A140AYW5
A	1331	LEU	-	expression tag	UNP A0A140AYW5
A	1332	LEU	-	expression tag	UNP A0A140AYW5
A	1333	SER	-	expression tag	UNP A0A140AYW5
A	1334	THR	-	expression tag	UNP A0A140AYW5
A	1335	PHE	-	expression tag	UNP A0A140AYW5
A	1336	LEU	-	expression tag	UNP A0A140AYW5
A	1337	GLY	-	expression tag	UNP A0A140AYW5
A	1338	HIS	-	expression tag	UNP A0A140AYW5
A	1339	HIS	-	expression tag	UNP A0A140AYW5
A	1340	HIS	-	expression tag	UNP A0A140AYW5
A	1341	HIS	-	expression tag	UNP A0A140AYW5
A	1342	HIS	-	expression tag	UNP A0A140AYW5
A	1343	HIS	-	expression tag	UNP A0A140AYW5
A	1344	HIS	-	expression tag	UNP A0A140AYW5
A	1345	HIS	-	expression tag	UNP A0A140AYW5
C	-13	MET	-	initiating methionine	UNP A0A140AYW5
C	-12	GLY	-	expression tag	UNP A0A140AYW5
C	-11	ILE	-	expression tag	UNP A0A140AYW5
C	-10	LEU	-	expression tag	UNP A0A140AYW5
C	-9	PRO	-	expression tag	UNP A0A140AYW5
C	-8	SER	-	expression tag	UNP A0A140AYW5
C	-7	PRO	-	expression tag	UNP A0A140AYW5
C	-6	GLY	-	expression tag	UNP A0A140AYW5
C	-5	MET	-	expression tag	UNP A0A140AYW5
C	-4	PRO	-	expression tag	UNP A0A140AYW5
C	-3	ALA	-	expression tag	UNP A0A140AYW5
C	-2	LEU	-	expression tag	UNP A0A140AYW5
C	-1	LEU	-	expression tag	UNP A0A140AYW5
C	0	SER	-	expression tag	UNP A0A140AYW5
C	1	LEU	-	expression tag	UNP A0A140AYW5
C	2	VAL	-	expression tag	UNP A0A140AYW5
C	3	SER	-	expression tag	UNP A0A140AYW5
C	4	LEU	-	expression tag	UNP A0A140AYW5
C	5	LEU	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	SER	-	expression tag	UNP A0A140AYW5
C	7	VAL	-	expression tag	UNP A0A140AYW5
C	8	LEU	-	expression tag	UNP A0A140AYW5
C	9	LEU	-	expression tag	UNP A0A140AYW5
C	10	MET	-	expression tag	UNP A0A140AYW5
C	11	GLY	-	expression tag	UNP A0A140AYW5
C	12	CYS	-	expression tag	UNP A0A140AYW5
C	13	VAL	-	expression tag	UNP A0A140AYW5
C	14	ALA	-	expression tag	UNP A0A140AYW5
C	15	GLU	-	expression tag	UNP A0A140AYW5
C	16	THR	-	expression tag	UNP A0A140AYW5
C	17	GLY	-	expression tag	UNP A0A140AYW5
C	18	THR	-	expression tag	UNP A0A140AYW5
C	529	ILE	THR	conflict	UNP A0A140AYW5
C	748	ALA	ARG	conflict	UNP A0A140AYW5
C	751	GLY	ARG	conflict	UNP A0A140AYW5
C	1020	GLN	ARG	conflict	UNP A0A140AYW5
C	1060	PRO	VAL	conflict	UNP A0A140AYW5
C	1061	PRO	LEU	conflict	UNP A0A140AYW5
C	1295	GLY	-	expression tag	UNP A0A140AYW5
C	1296	SER	-	expression tag	UNP A0A140AYW5
C	1297	GLY	-	expression tag	UNP A0A140AYW5
C	1298	ARG	-	expression tag	UNP A0A140AYW5
C	1299	GLU	-	expression tag	UNP A0A140AYW5
C	1300	ASN	-	expression tag	UNP A0A140AYW5
C	1301	LEU	-	expression tag	UNP A0A140AYW5
C	1302	TYR	-	expression tag	UNP A0A140AYW5
C	1303	PHE	-	expression tag	UNP A0A140AYW5
C	1304	GLN	-	expression tag	UNP A0A140AYW5
C	1305	GLY	-	expression tag	UNP A0A140AYW5
C	1306	GLY	-	expression tag	UNP A0A140AYW5
C	1307	GLY	-	expression tag	UNP A0A140AYW5
C	1308	GLY	-	expression tag	UNP A0A140AYW5
C	1309	SER	-	expression tag	UNP A0A140AYW5
C	1310	GLY	-	expression tag	UNP A0A140AYW5
C	1311	TYR	-	expression tag	UNP A0A140AYW5
C	1312	ILE	-	expression tag	UNP A0A140AYW5
C	1313	PRO	-	expression tag	UNP A0A140AYW5
C	1314	GLU	-	expression tag	UNP A0A140AYW5
C	1315	ALA	-	expression tag	UNP A0A140AYW5
C	1316	PRO	-	expression tag	UNP A0A140AYW5
C	1317	ARG	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1318	ASP	-	expression tag	UNP A0A140AYW5
C	1319	GLY	-	expression tag	UNP A0A140AYW5
C	1320	GLN	-	expression tag	UNP A0A140AYW5
C	1321	ALA	-	expression tag	UNP A0A140AYW5
C	1322	TYR	-	expression tag	UNP A0A140AYW5
C	1323	VAL	-	expression tag	UNP A0A140AYW5
C	1324	ARG	-	expression tag	UNP A0A140AYW5
C	1325	LYS	-	expression tag	UNP A0A140AYW5
C	1326	ASP	-	expression tag	UNP A0A140AYW5
C	1327	GLY	-	expression tag	UNP A0A140AYW5
C	1328	GLU	-	expression tag	UNP A0A140AYW5
C	1329	TRP	-	expression tag	UNP A0A140AYW5
C	1330	VAL	-	expression tag	UNP A0A140AYW5
C	1331	LEU	-	expression tag	UNP A0A140AYW5
C	1332	LEU	-	expression tag	UNP A0A140AYW5
C	1333	SER	-	expression tag	UNP A0A140AYW5
C	1334	THR	-	expression tag	UNP A0A140AYW5
C	1335	PHE	-	expression tag	UNP A0A140AYW5
C	1336	LEU	-	expression tag	UNP A0A140AYW5
C	1337	GLY	-	expression tag	UNP A0A140AYW5
C	1338	HIS	-	expression tag	UNP A0A140AYW5
C	1339	HIS	-	expression tag	UNP A0A140AYW5
C	1340	HIS	-	expression tag	UNP A0A140AYW5
C	1341	HIS	-	expression tag	UNP A0A140AYW5
C	1342	HIS	-	expression tag	UNP A0A140AYW5
C	1343	HIS	-	expression tag	UNP A0A140AYW5
C	1344	HIS	-	expression tag	UNP A0A140AYW5
C	1345	HIS	-	expression tag	UNP A0A140AYW5
E	-13	MET	-	initiating methionine	UNP A0A140AYW5
E	-12	GLY	-	expression tag	UNP A0A140AYW5
E	-11	ILE	-	expression tag	UNP A0A140AYW5
E	-10	LEU	-	expression tag	UNP A0A140AYW5
E	-9	PRO	-	expression tag	UNP A0A140AYW5
E	-8	SER	-	expression tag	UNP A0A140AYW5
E	-7	PRO	-	expression tag	UNP A0A140AYW5
E	-6	GLY	-	expression tag	UNP A0A140AYW5
E	-5	MET	-	expression tag	UNP A0A140AYW5
E	-4	PRO	-	expression tag	UNP A0A140AYW5
E	-3	ALA	-	expression tag	UNP A0A140AYW5
E	-2	LEU	-	expression tag	UNP A0A140AYW5
E	-1	LEU	-	expression tag	UNP A0A140AYW5
E	0	SER	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	LEU	-	expression tag	UNP A0A140AYW5
E	2	VAL	-	expression tag	UNP A0A140AYW5
E	3	SER	-	expression tag	UNP A0A140AYW5
E	4	LEU	-	expression tag	UNP A0A140AYW5
E	5	LEU	-	expression tag	UNP A0A140AYW5
E	6	SER	-	expression tag	UNP A0A140AYW5
E	7	VAL	-	expression tag	UNP A0A140AYW5
E	8	LEU	-	expression tag	UNP A0A140AYW5
E	9	LEU	-	expression tag	UNP A0A140AYW5
E	10	MET	-	expression tag	UNP A0A140AYW5
E	11	GLY	-	expression tag	UNP A0A140AYW5
E	12	CYS	-	expression tag	UNP A0A140AYW5
E	13	VAL	-	expression tag	UNP A0A140AYW5
E	14	ALA	-	expression tag	UNP A0A140AYW5
E	15	GLU	-	expression tag	UNP A0A140AYW5
E	16	THR	-	expression tag	UNP A0A140AYW5
E	17	GLY	-	expression tag	UNP A0A140AYW5
E	18	THR	-	expression tag	UNP A0A140AYW5
E	529	ILE	THR	conflict	UNP A0A140AYW5
E	748	ALA	ARG	conflict	UNP A0A140AYW5
E	751	GLY	ARG	conflict	UNP A0A140AYW5
E	1020	GLN	ARG	conflict	UNP A0A140AYW5
E	1060	PRO	VAL	conflict	UNP A0A140AYW5
E	1061	PRO	LEU	conflict	UNP A0A140AYW5
E	1295	GLY	-	expression tag	UNP A0A140AYW5
E	1296	SER	-	expression tag	UNP A0A140AYW5
E	1297	GLY	-	expression tag	UNP A0A140AYW5
E	1298	ARG	-	expression tag	UNP A0A140AYW5
E	1299	GLU	-	expression tag	UNP A0A140AYW5
E	1300	ASN	-	expression tag	UNP A0A140AYW5
E	1301	LEU	-	expression tag	UNP A0A140AYW5
E	1302	TYR	-	expression tag	UNP A0A140AYW5
E	1303	PHE	-	expression tag	UNP A0A140AYW5
E	1304	GLN	-	expression tag	UNP A0A140AYW5
E	1305	GLY	-	expression tag	UNP A0A140AYW5
E	1306	GLY	-	expression tag	UNP A0A140AYW5
E	1307	GLY	-	expression tag	UNP A0A140AYW5
E	1308	GLY	-	expression tag	UNP A0A140AYW5
E	1309	SER	-	expression tag	UNP A0A140AYW5
E	1310	GLY	-	expression tag	UNP A0A140AYW5
E	1311	TYR	-	expression tag	UNP A0A140AYW5
E	1312	ILE	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1313	PRO	-	expression tag	UNP A0A140AYW5
E	1314	GLU	-	expression tag	UNP A0A140AYW5
E	1315	ALA	-	expression tag	UNP A0A140AYW5
E	1316	PRO	-	expression tag	UNP A0A140AYW5
E	1317	ARG	-	expression tag	UNP A0A140AYW5
E	1318	ASP	-	expression tag	UNP A0A140AYW5
E	1319	GLY	-	expression tag	UNP A0A140AYW5
E	1320	GLN	-	expression tag	UNP A0A140AYW5
E	1321	ALA	-	expression tag	UNP A0A140AYW5
E	1322	TYR	-	expression tag	UNP A0A140AYW5
E	1323	VAL	-	expression tag	UNP A0A140AYW5
E	1324	ARG	-	expression tag	UNP A0A140AYW5
E	1325	LYS	-	expression tag	UNP A0A140AYW5
E	1326	ASP	-	expression tag	UNP A0A140AYW5
E	1327	GLY	-	expression tag	UNP A0A140AYW5
E	1328	GLU	-	expression tag	UNP A0A140AYW5
E	1329	TRP	-	expression tag	UNP A0A140AYW5
E	1330	VAL	-	expression tag	UNP A0A140AYW5
E	1331	LEU	-	expression tag	UNP A0A140AYW5
E	1332	LEU	-	expression tag	UNP A0A140AYW5
E	1333	SER	-	expression tag	UNP A0A140AYW5
E	1334	THR	-	expression tag	UNP A0A140AYW5
E	1335	PHE	-	expression tag	UNP A0A140AYW5
E	1336	LEU	-	expression tag	UNP A0A140AYW5
E	1337	GLY	-	expression tag	UNP A0A140AYW5
E	1338	HIS	-	expression tag	UNP A0A140AYW5
E	1339	HIS	-	expression tag	UNP A0A140AYW5
E	1340	HIS	-	expression tag	UNP A0A140AYW5
E	1341	HIS	-	expression tag	UNP A0A140AYW5
E	1342	HIS	-	expression tag	UNP A0A140AYW5
E	1343	HIS	-	expression tag	UNP A0A140AYW5
E	1344	HIS	-	expression tag	UNP A0A140AYW5
E	1345	HIS	-	expression tag	UNP A0A140AYW5

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4	Total	C	N	O	0	0
			50	28	2	20		
2	H	4	Total	C	N	O	0	0
			50	28	2	20		
2	N	4	Total	C	N	O	0	0
			50	28	2	20		
2	R	4	Total	C	N	O	0	0
			50	28	2	20		
2	X	4	Total	C	N	O	0	0
			50	28	2	20		
2	b	4	Total	C	N	O	0	0
			50	28	2	20		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		

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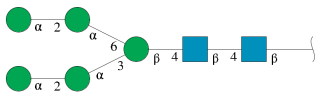
Mol	Chain	Residues	Atoms				AltConf	Trace
3	g	2	Total	C	N	O	0	0
			28	16	2	10		

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

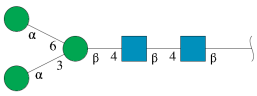


Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	7	Total	C	N	O	0	0
			83	46	2	35		
4	P	7	Total	C	N	O	0	0
			83	46	2	35		
4	Z	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 5 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.

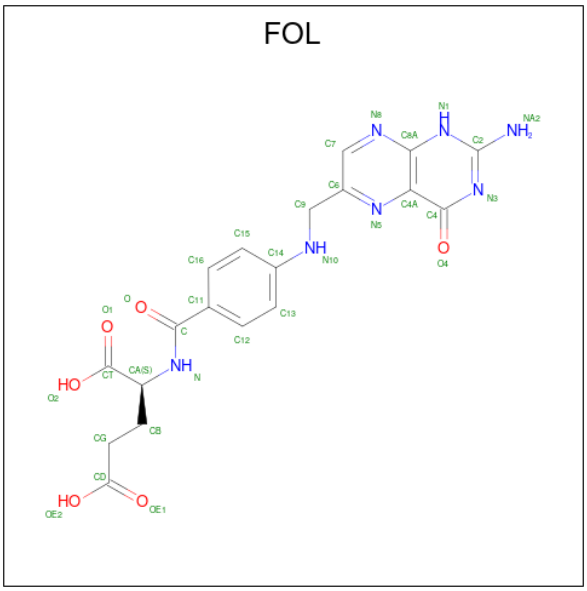
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	Q	3	Total	C	N	O	0	0
			39	22	2	15		
5	a	3	Total	C	N	O	0	0
			39	22	2	15		

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



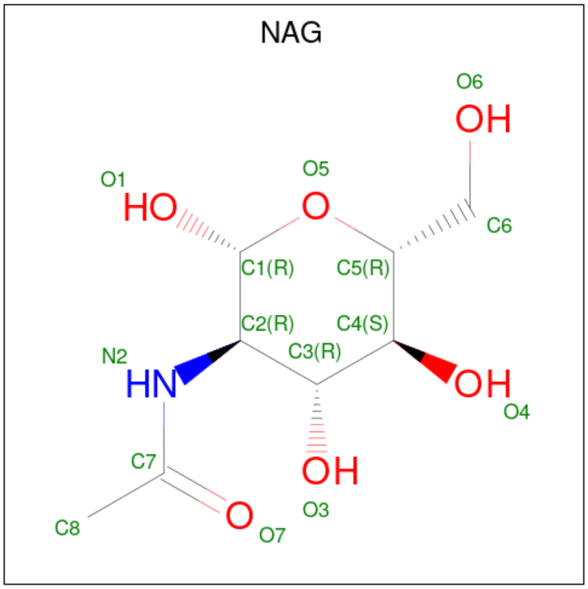
Mol	Chain	Residues	Atoms	AltConf	Trace
6	K	5	Total C N O 61 34 2 25	0	0
6	L	5	Total C N O 61 34 2 25	0	0
6	U	5	Total C N O 61 34 2 25	0	0
6	V	5	Total C N O 61 34 2 25	0	0
6	e	5	Total C N O 61 34 2 25	0	0
6	f	5	Total C N O 61 34 2 25	0	0

- Molecule 7 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O 32 19 7 6	0
7	C	1	Total C N O 32 19 7 6	0
7	E	1	Total C N O 32 19 7 6	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	C	1	Total C N O 14 8 1 5	0
8	C	1	Total C N O 14 8 1 5	0
8	C	1	Total C N O 14 8 1 5	0
8	C	1	Total C N O 14 8 1 5	0
8	C	1	Total C N O 14 8 1 5	0

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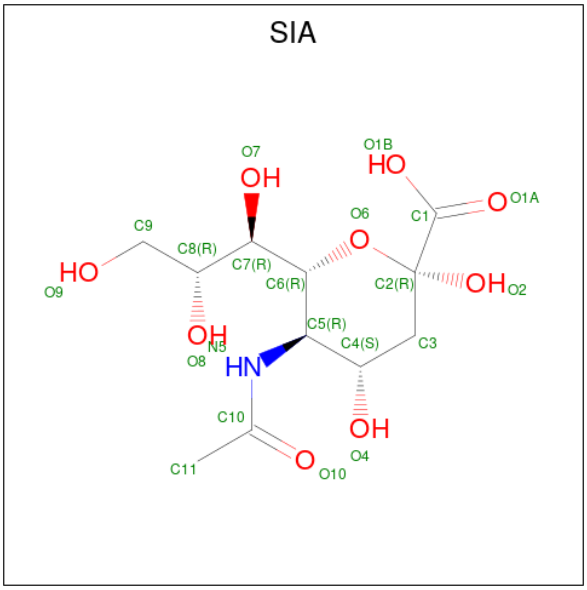
Mol	Chain	Residues	Atoms	AltConf
8	C	1	Total C N O 14 8 1 5	0
8	C	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 14 8 1 5	0

- Molecule 9 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



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

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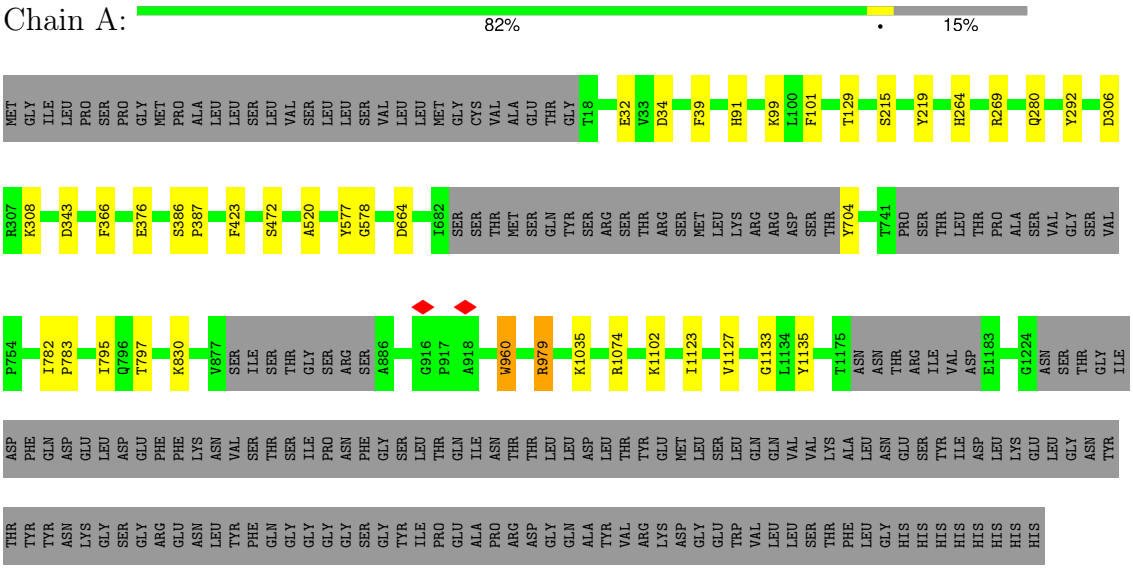
Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total	C	N	O	0
			21	11	1	9	

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.

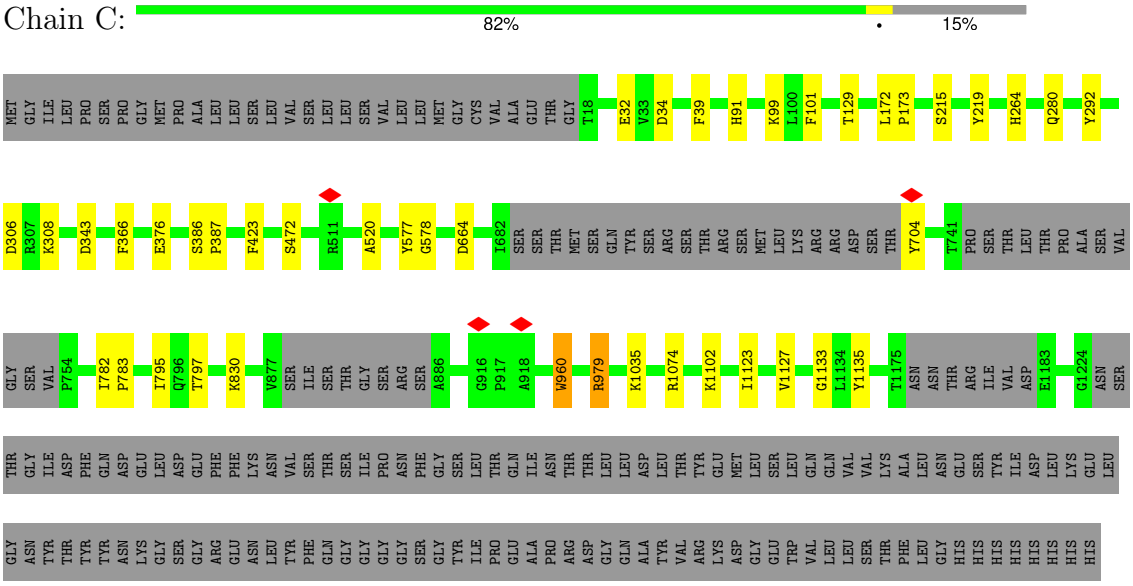
• Molecule 1: Spike glycoprotein

Chain A:



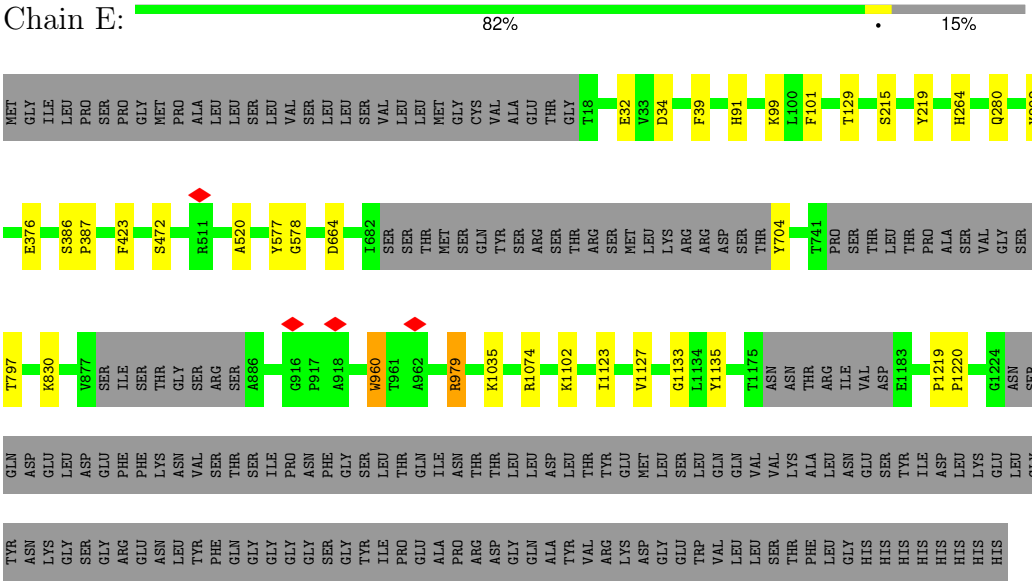
• Molecule 1: Spike glycoprotein

Chain C:



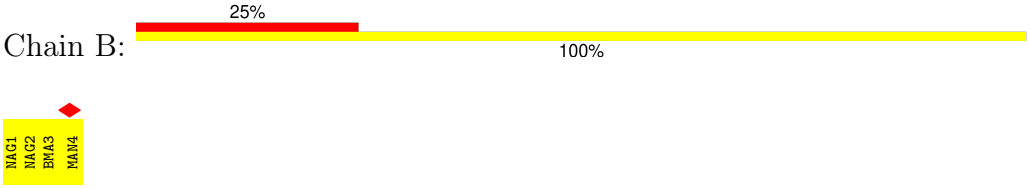
• Molecule 1: Spike glycoprotein

Chain E:



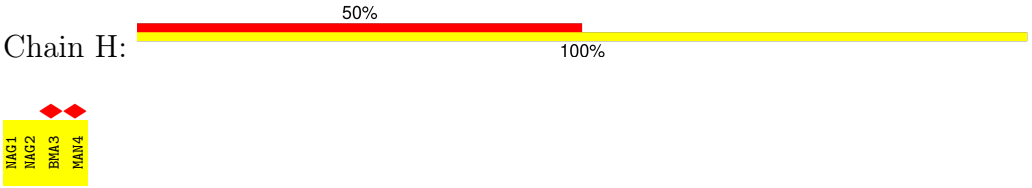
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



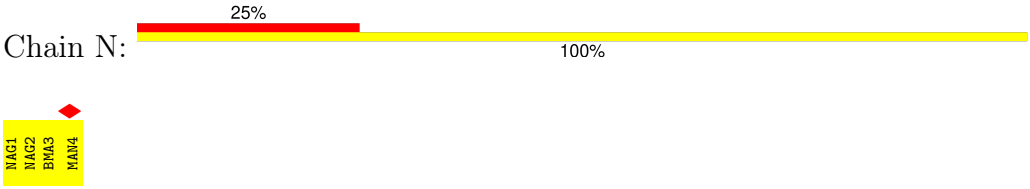
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



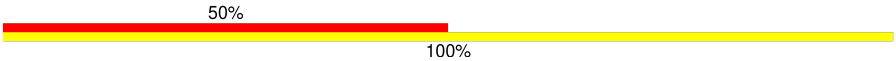
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

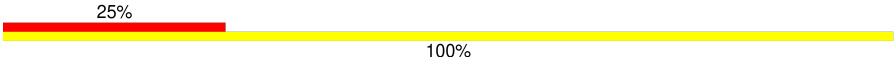


• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

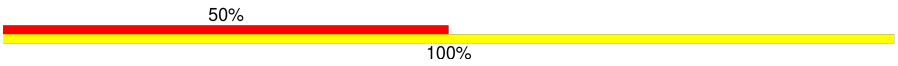
Chain R:



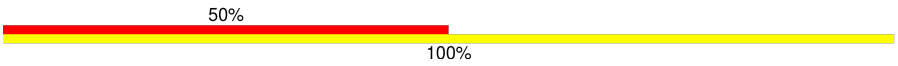
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

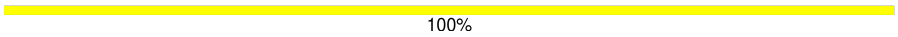
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

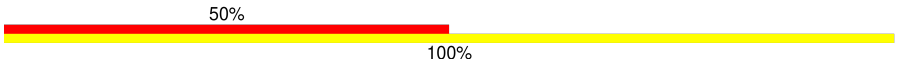
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

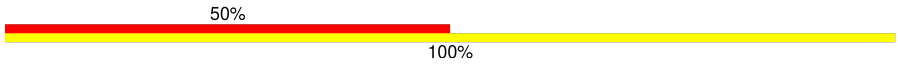
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

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

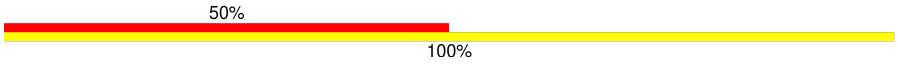
Chain J: 

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

Chain M: 

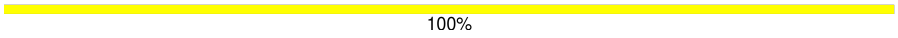
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain S:

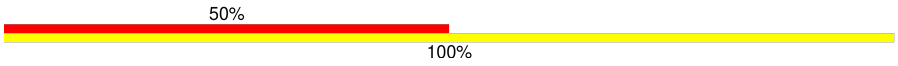


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

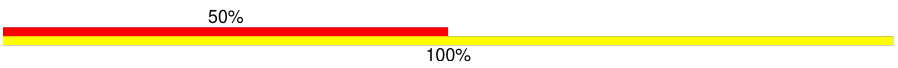
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



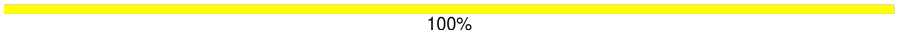
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



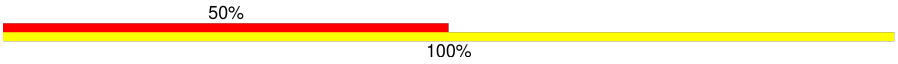
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



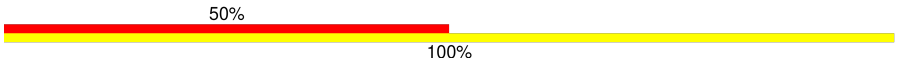
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



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

Chain g:



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

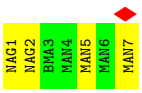
Chain F:

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

Chain P:

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

Chain Z:

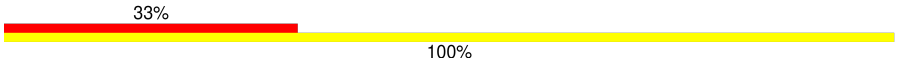


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

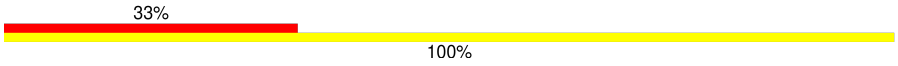
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



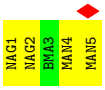
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



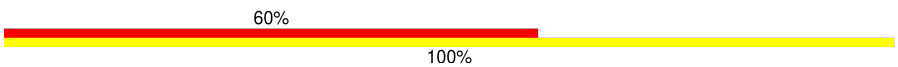
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:

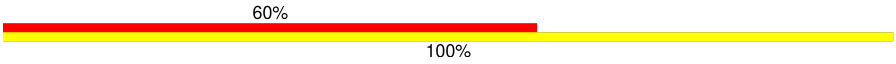


• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

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

Chain V:



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

Chain e:

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

Chain f:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	144792	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 ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.262	Depositor
Minimum map value	-3.457	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.93	6/9125 (0.1%)	0.72	7/12423 (0.1%)
1	C	0.93	6/9125 (0.1%)	0.72	6/12423 (0.0%)
1	E	0.93	6/9125 (0.1%)	0.73	6/12423 (0.0%)
All	All	0.93	18/27375 (0.1%)	0.73	19/37269 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	TYR	CB-CG	-5.77	1.43	1.51
1	C	292	TYR	CB-CG	-5.74	1.43	1.51
1	E	292	TYR	CB-CG	-5.73	1.43	1.51
1	E	1127	VAL	CB-CG2	-5.68	1.41	1.52
1	A	1127	VAL	CB-CG2	-5.68	1.41	1.52
1	C	1127	VAL	CB-CG2	-5.67	1.41	1.52
1	E	704	TYR	CG-CD1	5.25	1.46	1.39
1	A	704	TYR	CG-CD2	5.24	1.46	1.39
1	C	704	TYR	CG-CD1	5.24	1.46	1.39
1	C	704	TYR	CG-CD2	5.22	1.46	1.39
1	E	704	TYR	CG-CD2	5.21	1.46	1.39
1	A	704	TYR	CG-CD1	5.21	1.46	1.39
1	C	704	TYR	CE1-CZ	5.20	1.45	1.38
1	E	704	TYR	CE1-CZ	5.19	1.45	1.38
1	A	704	TYR	CE1-CZ	5.19	1.45	1.38
1	C	376	GLU	CD-OE2	-5.08	1.20	1.25
1	E	376	GLU	CD-OE2	-5.08	1.20	1.25
1	A	376	GLU	CD-OE2	-5.06	1.20	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	960	TRP	N-CA-CB	-8.15	95.92	110.60
1	A	960	TRP	N-CA-CB	-8.14	95.94	110.60
1	C	960	TRP	N-CA-CB	-8.13	95.96	110.60
1	E	960	TRP	N-CA-C	7.85	132.19	111.00
1	A	960	TRP	N-CA-C	7.83	132.14	111.00
1	C	960	TRP	N-CA-C	7.82	132.12	111.00
1	E	1135	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	C	1135	TYR	CB-CG-CD1	-5.98	117.41	121.00
1	A	1135	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	E	979	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	979	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	979	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	C	1074	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	1074	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	1074	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	577	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	E	577	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	577	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	269	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	8915	0	8590	22	0
1	C	8915	0	8590	23	0
1	E	8915	0	8590	21	0
2	B	50	0	43	0	0
2	H	50	0	43	0	0
2	N	50	0	43	0	0
2	R	50	0	43	0	0
2	X	50	0	43	0	0
2	b	50	0	43	0	0
3	D	28	0	25	0	0
3	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	0	0
3	M	28	0	25	0	0
3	O	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	W	28	0	25	0	0
3	Y	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	g	28	0	25	0	0
4	F	83	0	70	0	0
4	P	83	0	70	0	0
4	Z	83	0	70	0	0
5	G	39	0	34	0	0
5	Q	39	0	34	0	0
5	a	39	0	34	0	0
6	K	61	0	52	0	0
6	L	61	0	52	0	0
6	U	61	0	52	0	0
6	V	61	0	52	0	0
6	e	61	0	52	0	0
6	f	61	0	52	0	0
7	A	32	0	17	1	0
7	C	32	0	17	1	0
7	E	32	0	17	1	0
8	A	98	0	91	0	0
8	C	98	0	91	0	0
8	E	98	0	91	0	0
9	A	21	0	18	3	0
9	C	21	0	18	3	0
9	E	21	0	18	3	0
All	All	28566	0	27330	63	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 1.

All (63) 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:E:979:ARG:HD3	1:E:1123:ILE:O	1.72	0.90
1:A:979:ARG:HD3	1:A:1123:ILE:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:ARG:HD3	1:C:1123:ILE:O	1.72	0.88
1:C:215:SER:O	1:C:219:TYR:CE2	2.61	0.54
1:E:215:SER:O	1:E:219:TYR:CE2	2.61	0.54
1:A:215:SER:O	1:A:219:TYR:CE2	2.61	0.54
1:A:91:HIS:CD2	1:A:99:LYS:HE3	2.44	0.52
1:C:91:HIS:CD2	1:C:99:LYS:HE3	2.44	0.52
1:E:343:ASP:N	1:E:343:ASP:OD1	2.43	0.52
1:E:472:SER:HA	1:E:520:ALA:HB1	1.92	0.51
1:A:472:SER:HA	1:A:520:ALA:HB1	1.92	0.51
1:E:39:PHE:CE2	9:E:1409:SIA:H113	2.46	0.51
1:E:91:HIS:CD2	1:E:99:LYS:HE3	2.44	0.51
1:A:101:PHE:CZ	9:A:1409:SIA:C11	2.94	0.50
1:C:101:PHE:CZ	9:C:1409:SIA:C11	2.94	0.50
1:A:39:PHE:CE2	9:A:1409:SIA:H113	2.46	0.50
1:A:343:ASP:OD1	1:A:343:ASP:N	2.43	0.50
1:E:34:ASP:HB2	1:E:99:LYS:HE3	1.93	0.50
1:C:39:PHE:CE2	9:C:1409:SIA:H113	2.46	0.50
1:C:343:ASP:OD1	1:C:343:ASP:N	2.43	0.50
1:E:101:PHE:CZ	9:E:1409:SIA:C11	2.94	0.50
1:A:34:ASP:HB2	1:A:99:LYS:HE3	1.93	0.50
1:C:472:SER:HA	1:C:520:ALA:HB1	1.92	0.50
1:C:830:LYS:HD2	1:E:1035:LYS:HE2	1.94	0.49
1:A:830:LYS:HD2	1:C:1035:LYS:HE2	1.95	0.49
1:A:1035:LYS:HE2	1:E:830:LYS:HD2	1.95	0.49
1:C:34:ASP:HB2	1:C:99:LYS:HE3	1.94	0.48
1:E:795:ILE:HD11	1:E:1102:LYS:HD2	1.95	0.48
1:A:795:ILE:HD11	1:A:1102:LYS:HD2	1.95	0.48
1:C:795:ILE:HD11	1:C:1102:LYS:HD2	1.95	0.47
1:E:34:ASP:HB2	1:E:99:LYS:CE	2.44	0.47
1:C:34:ASP:HB2	1:C:99:LYS:CE	2.44	0.47
1:A:34:ASP:HB2	1:A:99:LYS:CE	2.44	0.46
1:A:664:ASP:OD1	1:A:664:ASP:C	2.56	0.44
1:E:664:ASP:OD1	1:E:664:ASP:C	2.56	0.43
1:E:39:PHE:CZ	9:E:1409:SIA:H113	2.53	0.43
1:A:39:PHE:CZ	9:A:1409:SIA:H113	2.54	0.43
1:C:664:ASP:C	1:C:664:ASP:OD1	2.56	0.43
1:C:39:PHE:CZ	9:C:1409:SIA:H113	2.54	0.43
1:A:782:ILE:HA	1:A:783:PRO:HD3	1.90	0.43
1:C:172:LEU:HA	1:C:173:PRO:HD2	1.93	0.43
1:E:264:HIS:ND1	1:E:280:GLN:NE2	2.67	0.42
1:A:797:THR:OG1	1:A:1133:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:ND1	1:A:280:GLN:NE2	2.67	0.42
1:A:32:GLU:O	1:A:99:LYS:HB2	2.20	0.42
1:C:32:GLU:O	1:C:99:LYS:HB2	2.19	0.42
1:C:386:SER:N	1:C:387:PRO:CD	2.83	0.42
1:E:32:GLU:O	1:E:99:LYS:HB2	2.20	0.42
1:C:264:HIS:ND1	1:C:280:GLN:NE2	2.67	0.41
1:E:386:SER:N	1:E:387:PRO:CD	2.83	0.41
1:C:797:THR:OG1	1:C:1133:GLY:HA2	2.19	0.41
1:C:215:SER:O	1:C:219:TYR:CD2	2.74	0.41
1:E:797:THR:OG1	1:E:1133:GLY:HA2	2.19	0.41
1:A:386:SER:N	1:A:387:PRO:CD	2.83	0.41
1:C:306:ASP:OD1	1:C:308:LYS:NZ	2.54	0.41
1:E:129:THR:H	7:E:1401:FOL:HN1	1.68	0.41
1:A:306:ASP:OD1	1:A:308:LYS:NZ	2.54	0.41
1:C:782:ILE:HA	1:C:783:PRO:HD3	1.91	0.41
1:A:215:SER:O	1:A:219:TYR:CD2	2.74	0.40
1:E:215:SER:O	1:E:219:TYR:CD2	2.74	0.40
1:C:129:THR:H	7:C:1401:FOL:HN1	1.68	0.40
1:A:129:THR:H	7:A:1401:FOL:HN1	1.68	0.40
1:E:1219:PRO:HA	1:E:1220:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1149/1359 (84%)	1127 (98%)	21 (2%)	1 (0%)	48	69
1	C	1149/1359 (84%)	1127 (98%)	21 (2%)	1 (0%)	48	69
1	E	1149/1359 (84%)	1127 (98%)	21 (2%)	1 (0%)	48	69
All	All	3447/4077 (84%)	3381 (98%)	63 (2%)	3 (0%)	50	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLY
1	C	578	GLY
1	E	578	GLY

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	983/1167 (84%)	980 (100%)	3 (0%)	91	97
1	C	983/1167 (84%)	980 (100%)	3 (0%)	91	97
1	E	983/1167 (84%)	980 (100%)	3 (0%)	91	97
All	All	2949/3501 (84%)	2940 (100%)	9 (0%)	90	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	PHE
1	A	423	PHE
1	A	960	TRP
1	C	366	PHE
1	C	423	PHE
1	C	960	TRP
1	E	366	PHE
1	E	423	PHE
1	E	960	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	C	280	GLN
1	E	280	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

108 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	B	1	1,2	14,14,15	1.34	1 (7%)	17,19,21	1.15	1 (5%)
2	NAG	B	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.79	0
2	BMA	B	3	2	11,11,12	0.59	0	15,15,17	0.73	1 (6%)
2	MAN	B	4	2	11,11,12	1.36	1 (9%)	15,15,17	0.56	0
3	NAG	D	1	1,3	14,14,15	1.59	2 (14%)	17,19,21	1.15	1 (5%)
3	NAG	D	2	3	14,14,15	1.45	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	F	1	4,1	14,14,15	1.34	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	F	2	4	14,14,15	1.41	2 (14%)	17,19,21	0.92	1 (5%)
4	BMA	F	3	4	11,11,12	1.01	0	15,15,17	0.58	0
4	MAN	F	4	4	11,11,12	0.72	0	15,15,17	0.71	0
4	MAN	F	5	4	11,11,12	1.40	2 (18%)	15,15,17	0.61	0
4	MAN	F	6	4	11,11,12	0.59	0	15,15,17	0.66	0
4	MAN	F	7	4	11,11,12	1.43	3 (27%)	15,15,17	0.54	0
5	NAG	G	1	1,5	14,14,15	1.48	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	G	2	5	14,14,15	1.49	2 (14%)	17,19,21	0.81	1 (5%)
5	BMA	G	3	5	11,11,12	1.40	3 (27%)	15,15,17	0.54	0
2	NAG	H	1	1,2	14,14,15	1.72	2 (14%)	17,19,21	1.07	1 (5%)
2	NAG	H	2	2	14,14,15	1.51	2 (14%)	17,19,21	0.96	1 (5%)
2	BMA	H	3	2	11,11,12	0.77	0	15,15,17	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	H	4	2	11,11,12	1.41	3 (27%)	15,15,17	0.52	0
3	NAG	I	1	1,3	14,14,15	1.46	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	I	2	3	14,14,15	1.46	2 (14%)	17,19,21	0.83	1 (5%)
3	NAG	J	1	1,3	14,14,15	1.56	2 (14%)	17,19,21	0.97	1 (5%)
3	NAG	J	2	3	14,14,15	1.51	2 (14%)	17,19,21	0.85	1 (5%)
6	NAG	K	1	1,6	14,14,15	1.35	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	K	2	6	14,14,15	1.43	1 (7%)	17,19,21	0.91	1 (5%)
6	BMA	K	3	6	11,11,12	1.00	0	15,15,17	0.62	0
6	MAN	K	4	6	11,11,12	1.40	3 (27%)	15,15,17	0.52	0
6	MAN	K	5	6	11,11,12	1.33	2 (18%)	15,15,17	0.54	0
6	NAG	L	1	1,6	14,14,15	1.38	1 (7%)	17,19,21	1.06	1 (5%)
6	NAG	L	2	6	14,14,15	1.48	2 (14%)	17,19,21	0.88	1 (5%)
6	BMA	L	3	6	11,11,12	1.09	1 (9%)	15,15,17	0.58	0
6	MAN	L	4	6	11,11,12	1.40	3 (27%)	15,15,17	0.55	0
6	MAN	L	5	6	11,11,12	1.39	2 (18%)	15,15,17	0.54	0
3	NAG	M	1	1,3	14,14,15	1.49	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	M	2	3	14,14,15	1.52	2 (14%)	17,19,21	0.86	1 (5%)
2	NAG	N	1	1,2	14,14,15	1.34	1 (7%)	17,19,21	1.15	1 (5%)
2	NAG	N	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.79	0
2	BMA	N	3	2	11,11,12	0.59	0	15,15,17	0.73	1 (6%)
2	MAN	N	4	2	11,11,12	1.37	1 (9%)	15,15,17	0.56	0
3	NAG	O	1	1,3	14,14,15	1.60	2 (14%)	17,19,21	1.15	1 (5%)
3	NAG	O	2	3	14,14,15	1.45	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	P	1	4,1	14,14,15	1.35	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	P	2	4	14,14,15	1.40	2 (14%)	17,19,21	0.92	1 (5%)
4	BMA	P	3	4	11,11,12	1.02	0	15,15,17	0.58	0
4	MAN	P	4	4	11,11,12	0.74	0	15,15,17	0.71	0
4	MAN	P	5	4	11,11,12	1.40	2 (18%)	15,15,17	0.60	0
4	MAN	P	6	4	11,11,12	0.60	0	15,15,17	0.66	0
4	MAN	P	7	4	11,11,12	1.43	3 (27%)	15,15,17	0.54	0
5	NAG	Q	1	1,5	14,14,15	1.49	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	Q	2	5	14,14,15	1.49	2 (14%)	17,19,21	0.81	1 (5%)
5	BMA	Q	3	5	11,11,12	1.40	3 (27%)	15,15,17	0.53	0
2	NAG	R	1	1,2	14,14,15	1.72	2 (14%)	17,19,21	1.07	1 (5%)
2	NAG	R	2	2	14,14,15	1.51	2 (14%)	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	R	3	2	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
2	MAN	R	4	2	11,11,12	1.40	2 (18%)	15,15,17	0.52	0
3	NAG	S	1	1,3	14,14,15	1.46	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	S	2	3	14,14,15	1.46	2 (14%)	17,19,21	0.83	1 (5%)
3	NAG	T	1	1,3	14,14,15	1.57	2 (14%)	17,19,21	0.96	1 (5%)
3	NAG	T	2	3	14,14,15	1.51	2 (14%)	17,19,21	0.86	1 (5%)
6	NAG	U	1	1,6	14,14,15	1.35	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	U	2	6	14,14,15	1.43	1 (7%)	17,19,21	0.90	1 (5%)
6	BMA	U	3	6	11,11,12	1.00	0	15,15,17	0.61	0
6	MAN	U	4	6	11,11,12	1.40	3 (27%)	15,15,17	0.53	0
6	MAN	U	5	6	11,11,12	1.34	2 (18%)	15,15,17	0.54	0
6	NAG	V	1	1,6	14,14,15	1.38	1 (7%)	17,19,21	1.05	1 (5%)
6	NAG	V	2	6	14,14,15	1.48	2 (14%)	17,19,21	0.88	1 (5%)
6	BMA	V	3	6	11,11,12	1.09	1 (9%)	15,15,17	0.57	0
6	MAN	V	4	6	11,11,12	1.40	3 (27%)	15,15,17	0.56	0
6	MAN	V	5	6	11,11,12	1.39	2 (18%)	15,15,17	0.54	0
3	NAG	W	1	1,3	14,14,15	1.49	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	W	2	3	14,14,15	1.51	2 (14%)	17,19,21	0.86	1 (5%)
2	NAG	X	1	1,2	14,14,15	1.33	1 (7%)	17,19,21	1.14	1 (5%)
2	NAG	X	2	2	14,14,15	1.25	2 (14%)	17,19,21	0.78	0
2	BMA	X	3	2	11,11,12	0.59	0	15,15,17	0.73	1 (6%)
2	MAN	X	4	2	11,11,12	1.36	1 (9%)	15,15,17	0.56	0
3	NAG	Y	1	1,3	14,14,15	1.58	2 (14%)	17,19,21	1.15	1 (5%)
3	NAG	Y	2	3	14,14,15	1.45	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	Z	1	4,1	14,14,15	1.34	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	Z	2	4	14,14,15	1.41	2 (14%)	17,19,21	0.92	1 (5%)
4	BMA	Z	3	4	11,11,12	1.00	0	15,15,17	0.58	0
4	MAN	Z	4	4	11,11,12	0.72	0	15,15,17	0.71	0
4	MAN	Z	5	4	11,11,12	1.40	2 (18%)	15,15,17	0.61	0
4	MAN	Z	6	4	11,11,12	0.59	0	15,15,17	0.66	0
4	MAN	Z	7	4	11,11,12	1.43	3 (27%)	15,15,17	0.54	0
5	NAG	a	1	1,5	14,14,15	1.48	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	a	2	5	14,14,15	1.49	2 (14%)	17,19,21	0.81	1 (5%)
5	BMA	a	3	5	11,11,12	1.40	3 (27%)	15,15,17	0.54	0
2	NAG	b	1	1,2	14,14,15	1.71	2 (14%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	b	2	2	14,14,15	1.51	2 (14%)	17,19,21	0.96	1 (5%)
2	BMA	b	3	2	11,11,12	0.78	0	15,15,17	0.95	1 (6%)
2	MAN	b	4	2	11,11,12	1.40	2 (18%)	15,15,17	0.52	0
3	NAG	c	1	1,3	14,14,15	1.46	1 (7%)	17,19,21	1.07	1 (5%)
3	NAG	c	2	3	14,14,15	1.46	2 (14%)	17,19,21	0.83	1 (5%)
3	NAG	d	1	1,3	14,14,15	1.55	2 (14%)	17,19,21	0.96	1 (5%)
3	NAG	d	2	3	14,14,15	1.50	2 (14%)	17,19,21	0.85	1 (5%)
6	NAG	e	1	1,6	14,14,15	1.36	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	e	2	6	14,14,15	1.42	1 (7%)	17,19,21	0.90	1 (5%)
6	BMA	e	3	6	11,11,12	1.00	0	15,15,17	0.61	0
6	MAN	e	4	6	11,11,12	1.40	3 (27%)	15,15,17	0.53	0
6	MAN	e	5	6	11,11,12	1.33	2 (18%)	15,15,17	0.54	0
6	NAG	f	1	1,6	14,14,15	1.38	1 (7%)	17,19,21	1.05	1 (5%)
6	NAG	f	2	6	14,14,15	1.48	2 (14%)	17,19,21	0.89	1 (5%)
6	BMA	f	3	6	11,11,12	1.09	1 (9%)	15,15,17	0.58	0
6	MAN	f	4	6	11,11,12	1.40	3 (27%)	15,15,17	0.55	0
6	MAN	f	5	6	11,11,12	1.39	2 (18%)	15,15,17	0.54	0
3	NAG	g	1	1,3	14,14,15	1.49	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	g	2	3	14,14,15	1.52	2 (14%)	17,19,21	0.85	1 (5%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	BMA	N	3	2	-	2/2/19/22	0/1/1/1
2	MAN	N	4	2	-	2/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	BMA	P	3	4	-	2/2/19/22	0/1/1/1
4	MAN	P	4	4	-	1/2/19/22	0/1/1/1
4	MAN	P	5	4	-	0/2/19/22	0/1/1/1
4	MAN	P	6	4	-	2/2/19/22	0/1/1/1
4	MAN	P	7	4	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	BMA	R	3	2	-	1/2/19/22	0/1/1/1
2	MAN	R	4	2	-	0/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	0/1/1/1
6	MAN	U	5	6	-	0/2/19/22	0/1/1/1
6	NAG	V	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	BMA	V	3	6	-	1/2/19/22	0/1/1/1
6	MAN	V	4	6	-	0/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	BMA	X	3	2	-	2/2/19/22	0/1/1/1
2	MAN	X	4	2	-	2/2/19/22	0/1/1/1
3	NAG	Y	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	1/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	2/2/19/22	0/1/1/1
4	MAN	Z	4	4	-	1/2/19/22	0/1/1/1
4	MAN	Z	5	4	-	0/2/19/22	0/1/1/1
4	MAN	Z	6	4	-	2/2/19/22	0/1/1/1
4	MAN	Z	7	4	-	0/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	BMA	b	3	2	-	1/2/19/22	0/1/1/1
2	MAN	b	4	2	-	0/2/19/22	0/1/1/1
3	NAG	c	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	d	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	0/6/23/26	0/1/1/1
6	NAG	e	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	BMA	e	3	6	-	2/2/19/22	0/1/1/1
6	MAN	e	4	6	-	0/2/19/22	0/1/1/1
6	MAN	e	5	6	-	0/2/19/22	0/1/1/1
6	NAG	f	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	0/6/23/26	0/1/1/1
6	BMA	f	3	6	-	1/2/19/22	0/1/1/1
6	MAN	f	4	6	-	0/2/19/22	0/1/1/1
6	MAN	f	5	6	-	0/2/19/22	0/1/1/1
3	NAG	g	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	g	2	3	-	0/6/23/26	0/1/1/1

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	1	NAG	C1-C2	5.04	1.59	1.52
2	H	1	NAG	C1-C2	5.04	1.59	1.52
2	b	1	NAG	C1-C2	5.01	1.59	1.52
3	O	1	NAG	C1-C2	4.40	1.58	1.52
3	D	1	NAG	C1-C2	4.36	1.58	1.52
3	Y	1	NAG	C1-C2	4.34	1.58	1.52
5	G	1	NAG	C1-C2	4.08	1.57	1.52
5	Q	1	NAG	C1-C2	4.08	1.57	1.52
3	g	2	NAG	C1-C2	4.07	1.57	1.52
3	T	1	NAG	C1-C2	4.07	1.57	1.52
5	a	1	NAG	C1-C2	4.06	1.57	1.52
3	M	2	NAG	C1-C2	4.06	1.57	1.52
3	M	1	NAG	C1-C2	4.04	1.57	1.52
3	J	1	NAG	C1-C2	4.04	1.57	1.52
3	W	2	NAG	C1-C2	4.04	1.57	1.52
6	f	1	NAG	C1-C2	4.04	1.57	1.52
3	g	1	NAG	C1-C2	4.02	1.57	1.52
6	L	1	NAG	C1-C2	4.02	1.57	1.52
3	W	1	NAG	C1-C2	4.02	1.57	1.52
6	V	1	NAG	C1-C2	4.02	1.57	1.52
3	I	1	NAG	C1-C2	4.01	1.57	1.52
3	d	1	NAG	C1-C2	4.01	1.57	1.52
3	c	1	NAG	C1-C2	3.99	1.57	1.52
3	S	1	NAG	C1-C2	3.98	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	NAG	C1-C2	3.93	1.57	1.52
6	e	1	NAG	C1-C2	3.93	1.57	1.52
3	T	2	NAG	C1-C2	3.92	1.57	1.52
6	K	1	NAG	C1-C2	3.91	1.57	1.52
3	d	2	NAG	C1-C2	3.90	1.57	1.52
6	U	1	NAG	C1-C2	3.89	1.57	1.52
6	K	2	NAG	C1-C2	3.82	1.57	1.52
3	I	2	NAG	C1-C2	3.81	1.57	1.52
6	e	2	NAG	C1-C2	3.81	1.57	1.52
6	U	2	NAG	C1-C2	3.81	1.57	1.52
3	c	2	NAG	C1-C2	3.80	1.57	1.52
3	S	2	NAG	C1-C2	3.80	1.57	1.52
2	R	2	NAG	C1-C2	3.75	1.57	1.52
4	F	2	NAG	C1-C2	3.73	1.57	1.52
2	b	2	NAG	C1-C2	3.73	1.57	1.52
4	Z	2	NAG	C1-C2	3.72	1.57	1.52
6	L	2	NAG	C1-C2	3.71	1.57	1.52
2	H	2	NAG	C1-C2	3.71	1.57	1.52
4	P	1	NAG	C1-C2	3.70	1.57	1.52
6	f	2	NAG	C1-C2	3.70	1.57	1.52
4	P	2	NAG	C1-C2	3.69	1.57	1.52
6	V	2	NAG	C1-C2	3.69	1.57	1.52
4	F	1	NAG	C1-C2	3.69	1.57	1.52
4	Z	1	NAG	C1-C2	3.69	1.57	1.52
5	G	2	NAG	C1-C2	3.67	1.57	1.52
3	Y	2	NAG	C1-C2	3.67	1.57	1.52
5	a	2	NAG	C1-C2	3.66	1.57	1.52
5	Q	2	NAG	C1-C2	3.66	1.57	1.52
3	D	2	NAG	C1-C2	3.66	1.57	1.52
3	O	2	NAG	C1-C2	3.64	1.57	1.52
2	X	1	NAG	C1-C2	3.57	1.57	1.52
2	B	1	NAG	C1-C2	3.57	1.57	1.52
2	N	1	NAG	C1-C2	3.57	1.57	1.52
2	N	2	NAG	C1-C2	3.31	1.56	1.52
2	B	2	NAG	C1-C2	3.29	1.56	1.52
2	X	2	NAG	C1-C2	3.28	1.56	1.52
4	Z	5	MAN	O5-C5	2.65	1.48	1.43
4	F	5	MAN	O5-C5	2.65	1.48	1.43
2	R	4	MAN	O5-C5	2.64	1.48	1.43
2	H	4	MAN	O5-C5	2.63	1.48	1.43
4	P	5	MAN	O5-C5	2.63	1.48	1.43
2	b	4	MAN	O5-C5	2.62	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	4	MAN	O5-C5	2.60	1.48	1.43
6	U	4	MAN	O5-C5	2.60	1.48	1.43
6	e	4	MAN	O5-C5	2.59	1.48	1.43
6	f	4	MAN	O5-C5	2.58	1.48	1.43
6	L	4	MAN	O5-C5	2.57	1.48	1.43
5	Q	3	BMA	O5-C5	2.56	1.48	1.43
4	Z	7	MAN	O5-C5	2.55	1.48	1.43
4	P	7	MAN	O5-C5	2.55	1.48	1.43
6	V	4	MAN	O5-C5	2.55	1.48	1.43
4	F	7	MAN	O5-C5	2.55	1.48	1.43
5	G	3	BMA	O5-C5	2.53	1.48	1.43
6	V	5	MAN	O5-C5	2.52	1.48	1.43
2	H	1	NAG	O5-C5	2.51	1.48	1.43
6	L	5	MAN	O5-C5	2.51	1.48	1.43
2	B	4	MAN	O5-C5	2.51	1.48	1.43
6	f	5	MAN	O5-C5	2.51	1.48	1.43
5	a	3	BMA	O5-C5	2.50	1.48	1.43
2	X	4	MAN	O5-C5	2.49	1.48	1.43
2	N	4	MAN	O5-C5	2.49	1.48	1.43
2	R	1	NAG	O5-C5	2.49	1.48	1.43
2	b	1	NAG	O5-C5	2.48	1.48	1.43
3	d	2	NAG	O5-C5	2.46	1.48	1.43
2	R	2	NAG	O5-C5	2.45	1.48	1.43
3	T	2	NAG	O5-C5	2.45	1.48	1.43
3	J	2	NAG	O5-C5	2.44	1.48	1.43
2	H	2	NAG	O5-C5	2.42	1.48	1.43
3	g	2	NAG	O5-C5	2.41	1.48	1.43
3	O	2	NAG	O5-C5	2.40	1.48	1.43
3	M	2	NAG	O5-C5	2.40	1.48	1.43
3	Y	2	NAG	O5-C5	2.40	1.48	1.43
3	D	2	NAG	O5-C5	2.40	1.48	1.43
6	e	5	MAN	O5-C5	2.40	1.48	1.43
6	U	5	MAN	O5-C5	2.40	1.48	1.43
2	b	2	NAG	O5-C5	2.39	1.48	1.43
6	K	5	MAN	O5-C5	2.38	1.48	1.43
3	W	2	NAG	O5-C5	2.38	1.48	1.43
3	c	2	NAG	O5-C5	2.31	1.47	1.43
3	I	2	NAG	O5-C5	2.30	1.47	1.43
5	Q	2	NAG	O5-C5	2.29	1.47	1.43
5	G	2	NAG	O5-C5	2.29	1.47	1.43
3	S	2	NAG	O5-C5	2.28	1.47	1.43
5	a	2	NAG	O5-C5	2.28	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C5	2.27	1.47	1.43
6	L	2	NAG	O5-C5	2.27	1.47	1.43
3	J	1	NAG	O5-C5	2.27	1.47	1.43
6	V	2	NAG	O5-C5	2.27	1.47	1.43
3	d	1	NAG	O5-C5	2.26	1.47	1.43
6	f	2	NAG	O5-C5	2.25	1.47	1.43
4	F	7	MAN	C1-C2	2.16	1.57	1.52
5	a	3	BMA	C2-C3	2.16	1.55	1.52
4	P	7	MAN	C1-C2	2.16	1.57	1.52
4	Z	7	MAN	C1-C2	2.14	1.57	1.52
4	P	7	MAN	C2-C3	2.14	1.55	1.52
4	F	7	MAN	C2-C3	2.13	1.55	1.52
6	U	4	MAN	C2-C3	2.13	1.55	1.52
4	Z	7	MAN	C2-C3	2.13	1.55	1.52
6	e	4	MAN	C2-C3	2.12	1.55	1.52
6	V	5	MAN	C2-C3	2.12	1.55	1.52
5	G	3	BMA	C1-C2	2.12	1.57	1.52
5	Q	3	BMA	C1-C2	2.12	1.57	1.52
5	Q	3	BMA	C2-C3	2.12	1.55	1.52
6	K	4	MAN	C2-C3	2.12	1.55	1.52
5	G	3	BMA	C2-C3	2.11	1.55	1.52
3	O	1	NAG	O5-C5	2.11	1.47	1.43
6	L	5	MAN	C2-C3	2.11	1.55	1.52
6	f	5	MAN	C2-C3	2.11	1.55	1.52
5	a	3	BMA	C1-C2	2.11	1.57	1.52
3	D	1	NAG	O5-C5	2.11	1.47	1.43
3	Y	1	NAG	O5-C5	2.10	1.47	1.43
4	Z	5	MAN	C2-C3	2.10	1.55	1.52
3	M	1	NAG	O5-C5	2.10	1.47	1.43
3	g	1	NAG	O5-C5	2.09	1.47	1.43
4	F	5	MAN	C2-C3	2.09	1.55	1.52
6	f	4	MAN	C2-C3	2.09	1.55	1.52
3	W	1	NAG	O5-C5	2.08	1.47	1.43
4	P	5	MAN	C2-C3	2.08	1.55	1.52
6	U	4	MAN	C1-C2	2.07	1.57	1.52
6	L	3	BMA	O5-C5	2.07	1.47	1.43
6	f	3	BMA	O5-C5	2.07	1.47	1.43
6	V	4	MAN	C1-C2	2.07	1.57	1.52
6	L	4	MAN	C2-C3	2.07	1.55	1.52
6	K	4	MAN	C1-C2	2.06	1.57	1.52
6	V	3	BMA	O5-C5	2.06	1.47	1.43
6	V	4	MAN	C2-C3	2.05	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	e	4	MAN	C1-C2	2.05	1.57	1.52
4	Z	2	NAG	O5-C5	2.05	1.47	1.43
2	X	2	NAG	O5-C5	2.04	1.47	1.43
6	L	4	MAN	C1-C2	2.04	1.57	1.52
2	N	2	NAG	O5-C5	2.04	1.47	1.43
6	f	4	MAN	C1-C2	2.04	1.57	1.52
2	B	2	NAG	O5-C5	2.04	1.47	1.43
6	K	5	MAN	C2-C3	2.04	1.55	1.52
4	P	2	NAG	O5-C5	2.03	1.47	1.43
6	U	5	MAN	C2-C3	2.03	1.55	1.52
2	b	4	MAN	C2-C3	2.02	1.55	1.52
6	e	5	MAN	C2-C3	2.02	1.55	1.52
4	F	2	NAG	O5-C5	2.01	1.47	1.43
2	H	4	MAN	C2-C3	2.01	1.55	1.52
2	H	4	MAN	C1-C2	2.01	1.57	1.52
2	R	4	MAN	C1-C2	2.00	1.57	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	1	NAG	O4-C4-C3	-2.73	103.94	110.38
2	H	1	NAG	O4-C4-C3	-2.73	103.94	110.38
2	b	1	NAG	O4-C4-C3	-2.72	103.97	110.38
3	S	1	NAG	C8-C7-N2	2.68	120.56	116.12
3	I	1	NAG	C8-C7-N2	2.65	120.52	116.12
3	c	1	NAG	C8-C7-N2	2.63	120.48	116.12
6	U	1	NAG	C8-C7-N2	2.45	120.19	116.12
6	K	1	NAG	C8-C7-N2	2.45	120.19	116.12
6	e	1	NAG	C8-C7-N2	2.45	120.17	116.12
4	F	2	NAG	C8-C7-N2	2.43	120.15	116.12
4	Z	2	NAG	C8-C7-N2	2.43	120.15	116.12
4	P	2	NAG	C8-C7-N2	2.42	120.13	116.12
3	Y	1	NAG	C8-C7-N2	2.40	120.10	116.12
3	D	1	NAG	C8-C7-N2	2.38	120.07	116.12
3	O	1	NAG	C8-C7-N2	2.38	120.06	116.12
3	W	2	NAG	C8-C7-N2	2.34	120.00	116.12
3	M	2	NAG	C8-C7-N2	2.34	119.99	116.12
6	K	2	NAG	C8-C7-N2	2.33	119.99	116.12
6	U	2	NAG	C8-C7-N2	2.33	119.98	116.12
3	g	2	NAG	C8-C7-N2	2.33	119.98	116.12
6	e	2	NAG	C8-C7-N2	2.33	119.98	116.12
4	P	1	NAG	C8-C7-N2	2.32	119.97	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	C8-C7-N2	2.31	119.95	116.12
4	Z	1	NAG	C8-C7-N2	2.31	119.95	116.12
2	N	1	NAG	C8-C7-N2	2.30	119.93	116.12
2	B	1	NAG	C8-C7-N2	2.30	119.93	116.12
3	D	2	NAG	C8-C7-N2	2.29	119.92	116.12
2	X	1	NAG	C8-C7-N2	2.29	119.91	116.12
3	Y	2	NAG	C8-C7-N2	2.28	119.91	116.12
6	f	2	NAG	C8-C7-N2	2.28	119.90	116.12
2	b	3	BMA	C2-C3-C4	-2.28	106.85	110.86
3	O	2	NAG	C8-C7-N2	2.28	119.90	116.12
2	R	3	BMA	C2-C3-C4	-2.28	106.85	110.86
3	J	2	NAG	C8-C7-N2	2.27	119.88	116.12
3	T	2	NAG	C8-C7-N2	2.26	119.87	116.12
6	L	2	NAG	C8-C7-N2	2.26	119.86	116.12
2	H	3	BMA	C2-C3-C4	-2.26	106.89	110.86
3	d	2	NAG	C8-C7-N2	2.26	119.86	116.12
6	V	2	NAG	C8-C7-N2	2.25	119.84	116.12
2	b	2	NAG	C8-C7-N2	2.24	119.84	116.12
6	V	1	NAG	C1-C2-N2	-2.24	106.90	110.43
2	H	2	NAG	C8-C7-N2	2.24	119.83	116.12
6	L	1	NAG	C1-C2-N2	-2.24	106.91	110.43
5	a	2	NAG	C8-C7-N2	2.23	119.82	116.12
6	f	1	NAG	C1-C2-N2	-2.23	106.92	110.43
2	R	2	NAG	C8-C7-N2	2.23	119.81	116.12
3	I	2	NAG	C8-C7-N2	2.22	119.80	116.12
5	G	2	NAG	C8-C7-N2	2.22	119.80	116.12
3	S	2	NAG	C8-C7-N2	2.22	119.79	116.12
3	c	2	NAG	C8-C7-N2	2.21	119.78	116.12
5	Q	2	NAG	C8-C7-N2	2.21	119.78	116.12
3	J	1	NAG	C8-C7-N2	2.14	119.66	116.12
3	d	1	NAG	C8-C7-N2	2.14	119.66	116.12
3	M	1	NAG	C8-C7-N2	2.12	119.64	116.12
3	T	1	NAG	C8-C7-N2	2.12	119.63	116.12
3	g	1	NAG	C8-C7-N2	2.11	119.62	116.12
3	W	1	NAG	C8-C7-N2	2.11	119.61	116.12
2	N	3	BMA	C2-C3-C4	-2.05	107.25	110.86
5	Q	1	NAG	C8-C7-N2	2.05	119.52	116.12
5	a	1	NAG	C8-C7-N2	2.05	119.51	116.12
2	B	3	BMA	C2-C3-C4	-2.04	107.27	110.86
2	X	3	BMA	C2-C3-C4	-2.04	107.28	110.86
5	G	1	NAG	C8-C7-N2	2.03	119.49	116.12
3	S	1	NAG	O7-C7-C8	-2.03	118.44	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	NAG	O7-C7-C8	-2.01	118.48	122.05

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	BMA	C4-C5-C6-O6
4	P	3	BMA	C4-C5-C6-O6
4	Z	3	BMA	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	e	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6
4	Z	3	BMA	O5-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
6	e	3	BMA	C4-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
4	P	6	MAN	O5-C5-C6-O6
4	Z	6	MAN	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	N	4	MAN	O5-C5-C6-O6
2	X	4	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	X	3	BMA	O5-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
6	f	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	R	3	BMA	O5-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
4	Z	4	MAN	O5-C5-C6-O6

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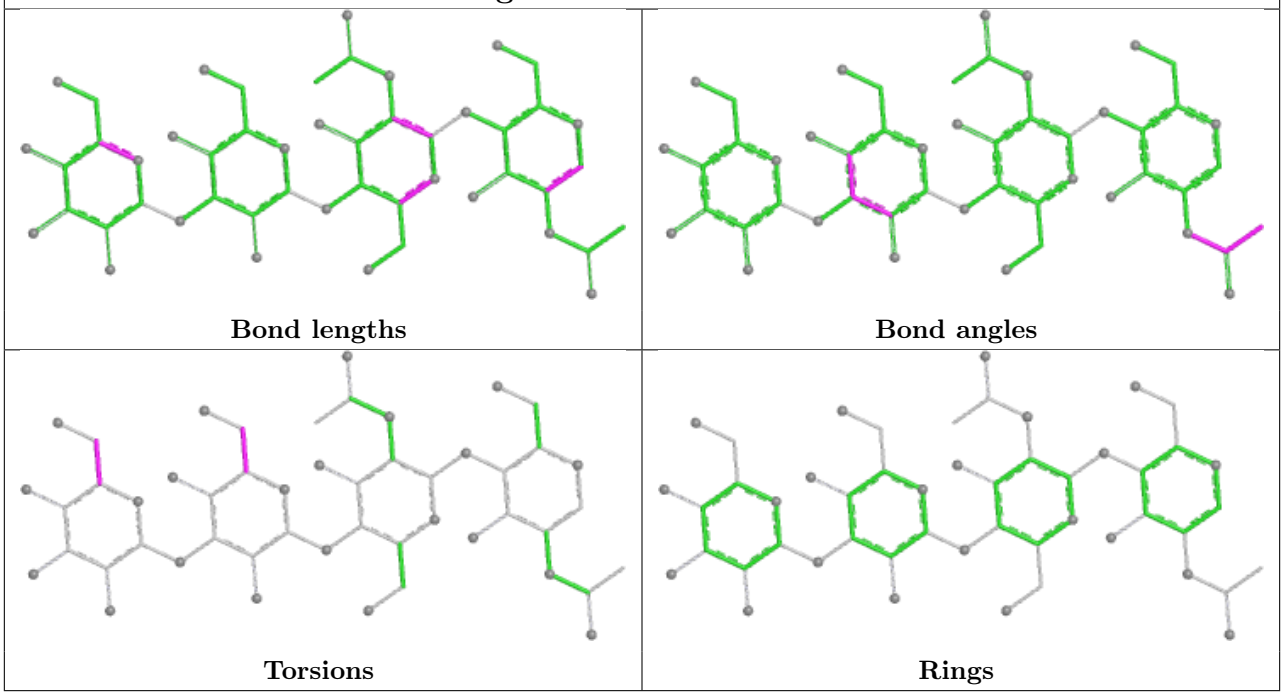
Mol	Chain	Res	Type	Atoms
4	P	6	MAN	C4-C5-C6-O6
4	F	6	MAN	C4-C5-C6-O6
4	Z	6	MAN	C4-C5-C6-O6
2	X	4	MAN	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	N	4	MAN	C4-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
4	P	2	NAG	C1-C2-N2-C7
4	Z	2	NAG	C1-C2-N2-C7
2	B	3	BMA	C4-C5-C6-O6
2	X	3	BMA	C4-C5-C6-O6
2	N	3	BMA	C4-C5-C6-O6

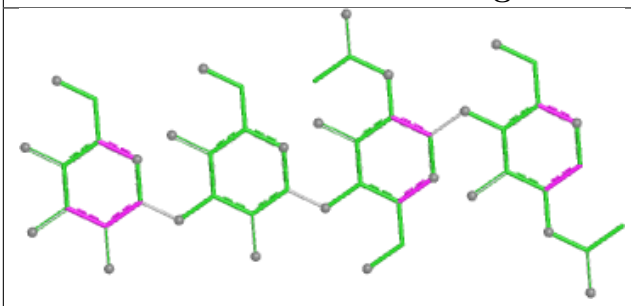
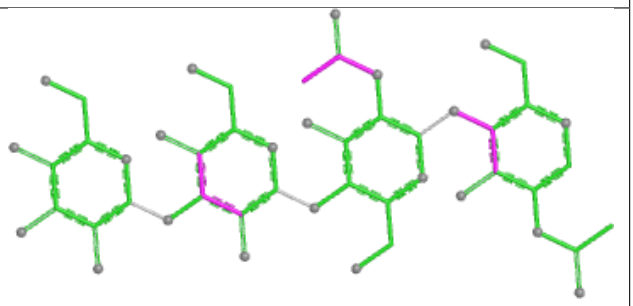
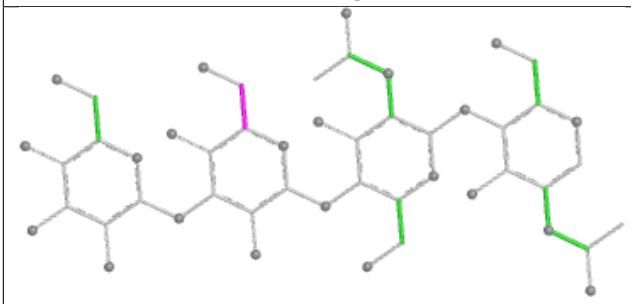
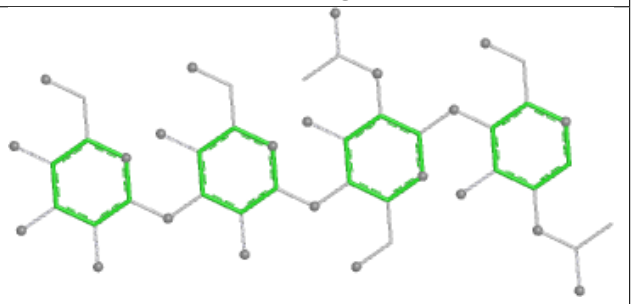
There are no ring outliers.

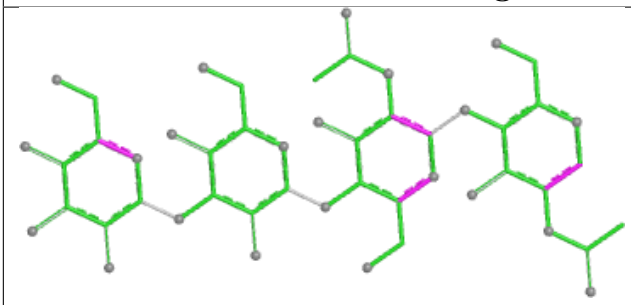
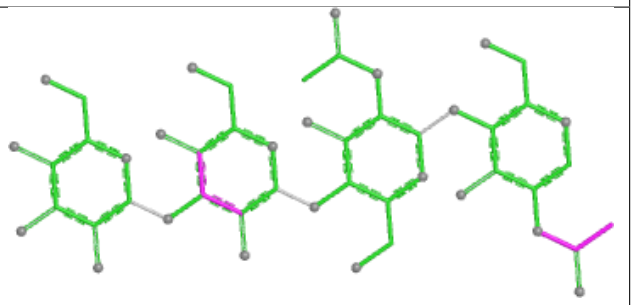
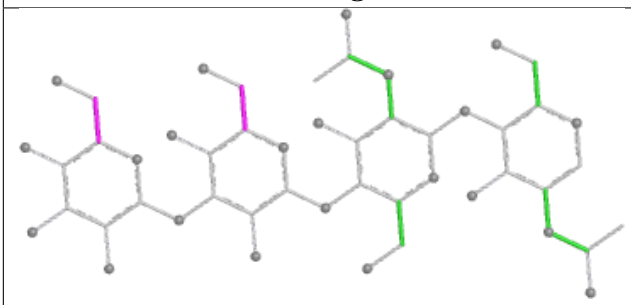
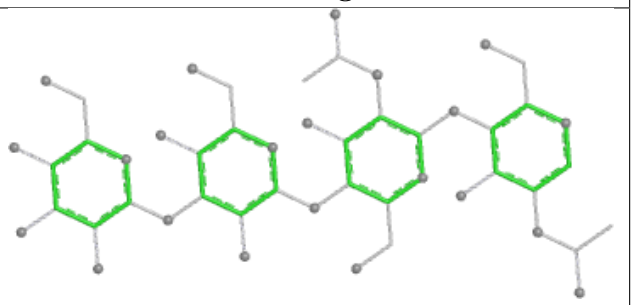
No monomer is involved in short contacts.

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

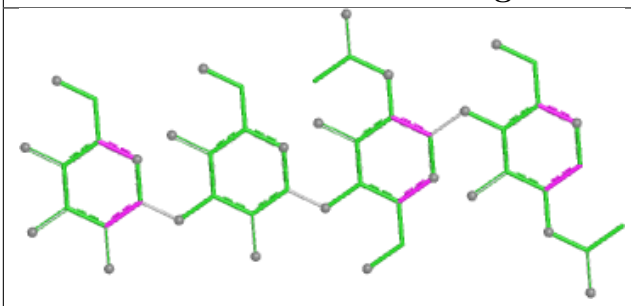
Oligosaccharide Chain B



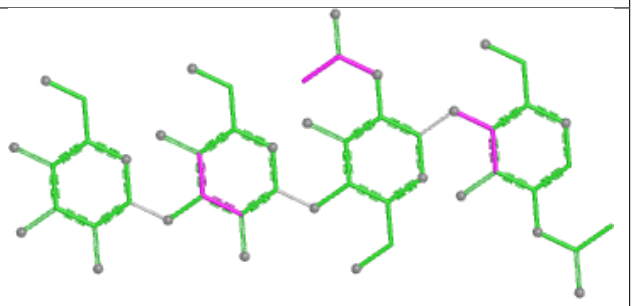
Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

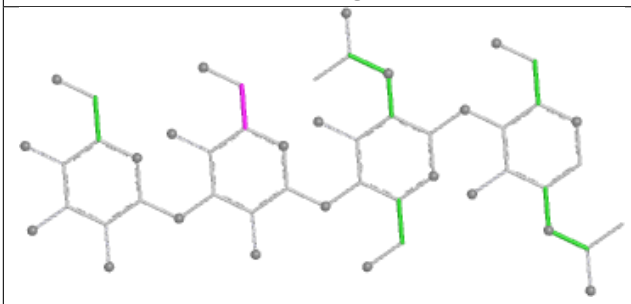
Oligosaccharide Chain R



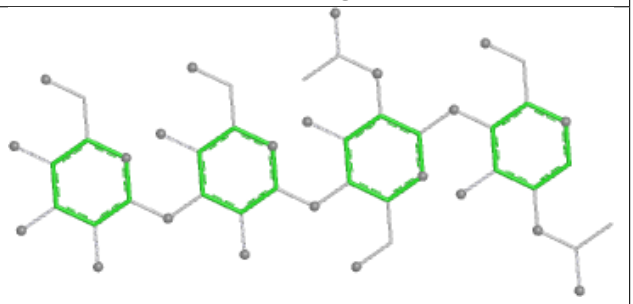
Bond lengths



Bond angles

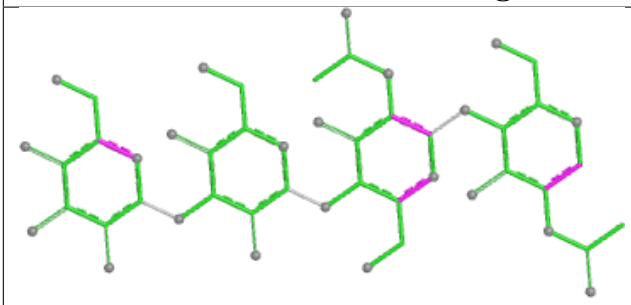


Torsions

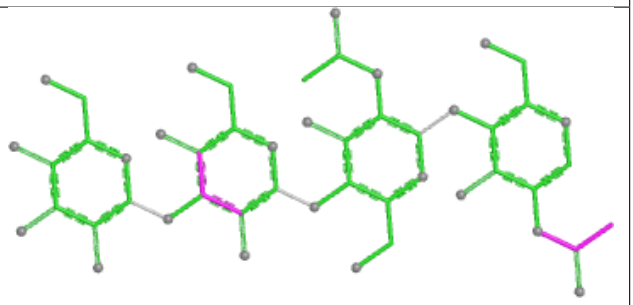


Rings

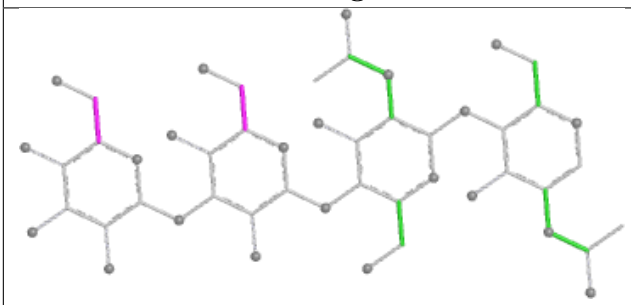
Oligosaccharide Chain X



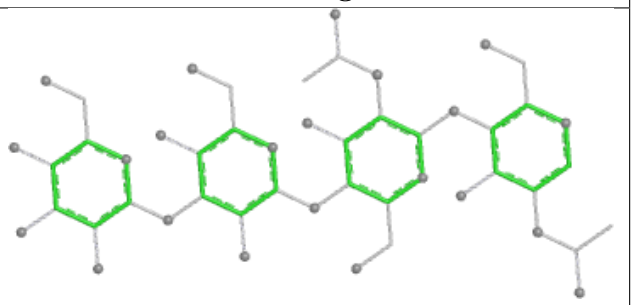
Bond lengths



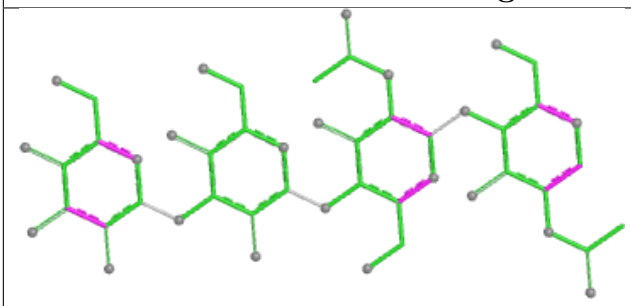
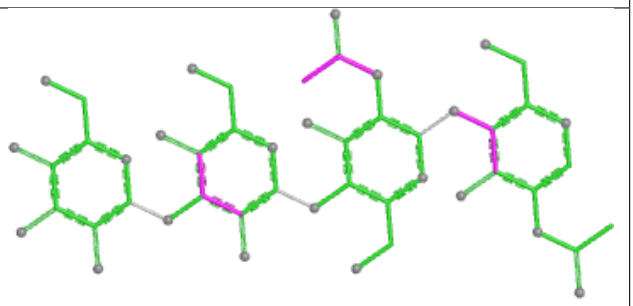
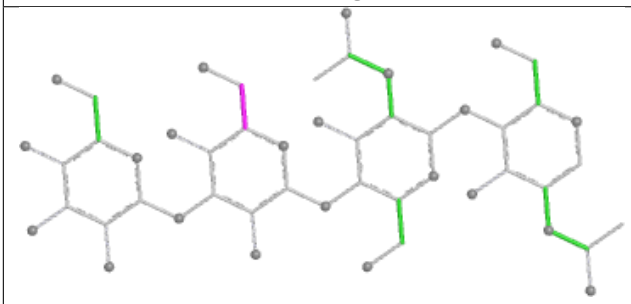
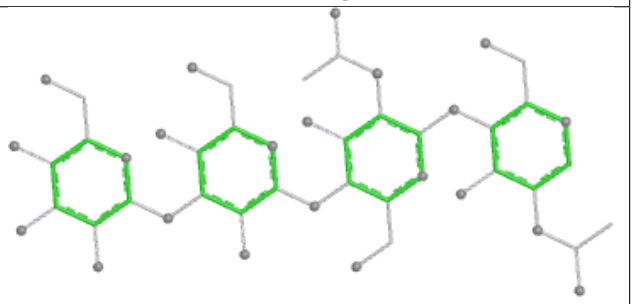
Bond angles



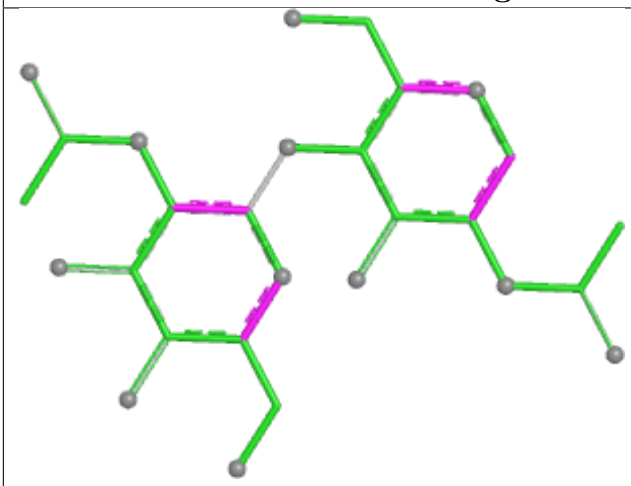
Torsions



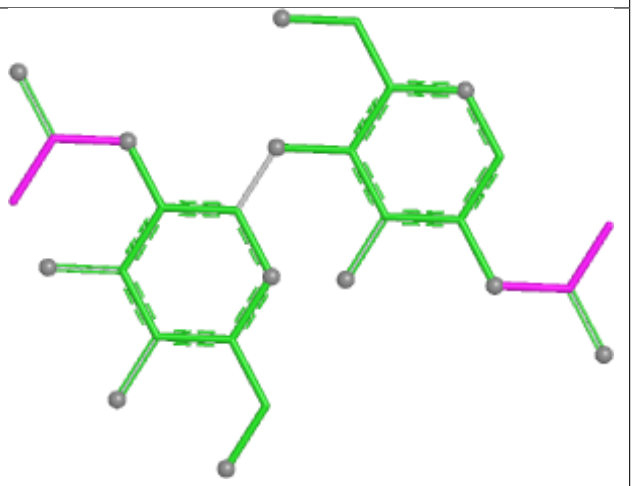
Rings

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

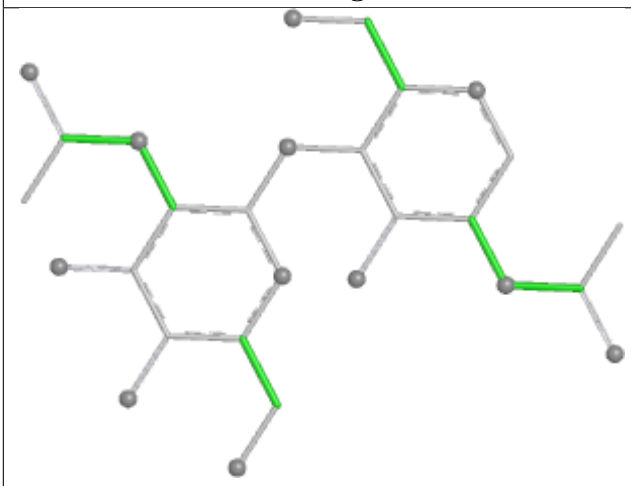
Oligosaccharide Chain D



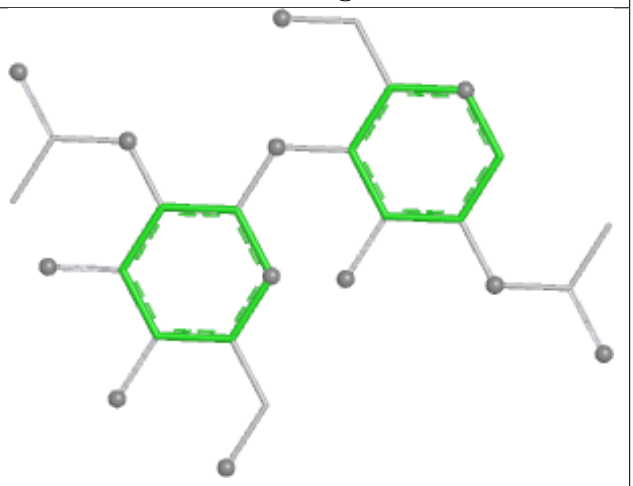
Bond lengths



Bond angles

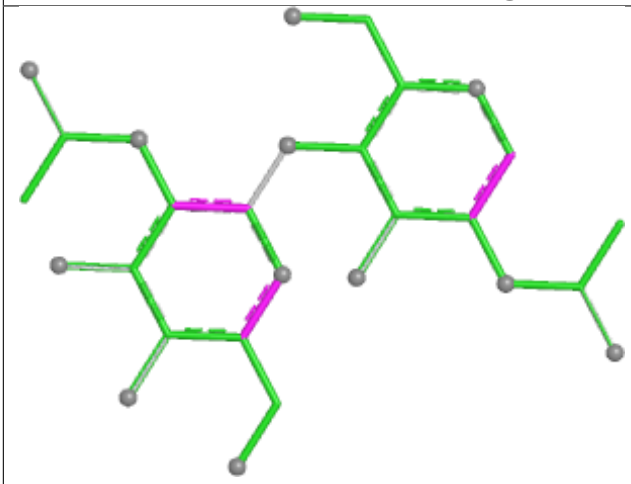


Torsions

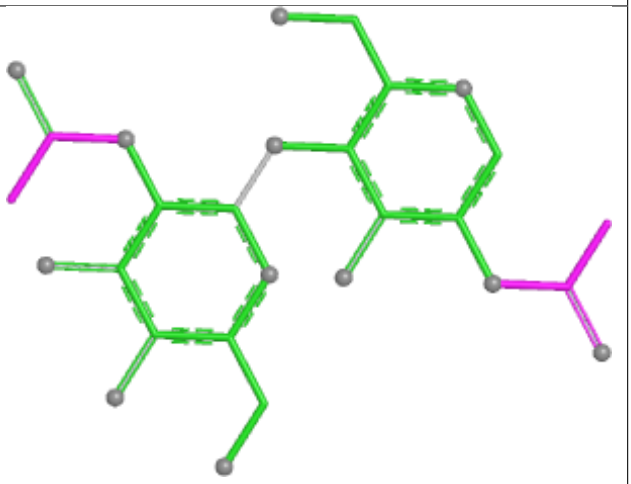


Rings

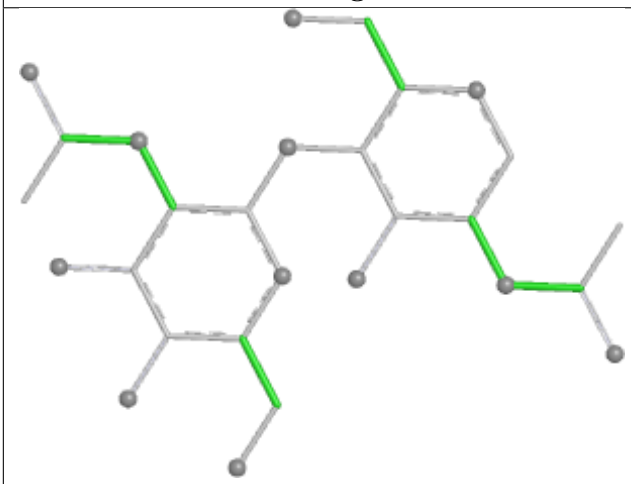
Oligosaccharide Chain I



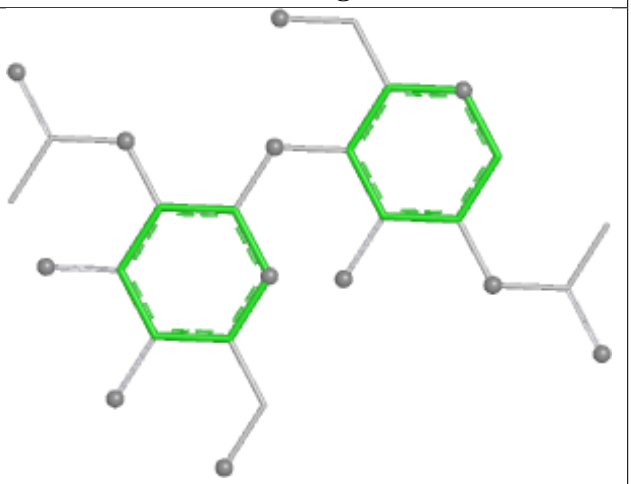
Bond lengths



Bond angles

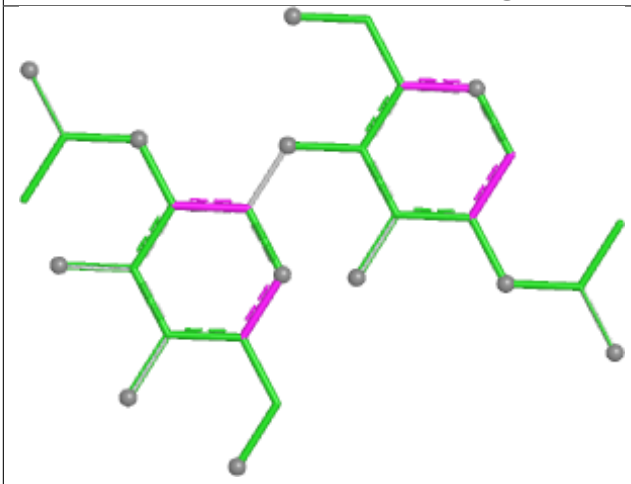


Torsions

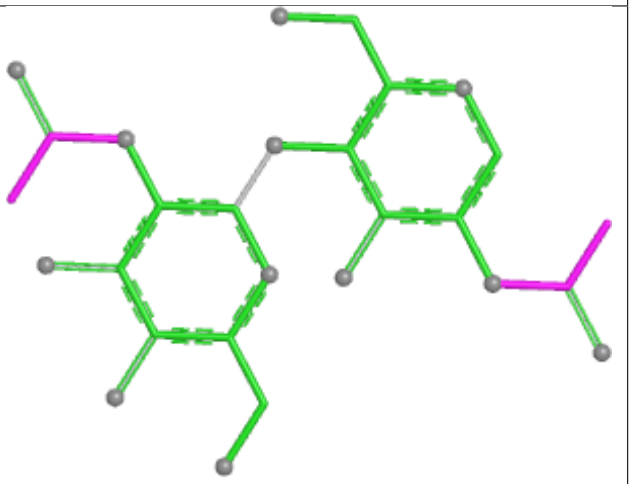


Rings

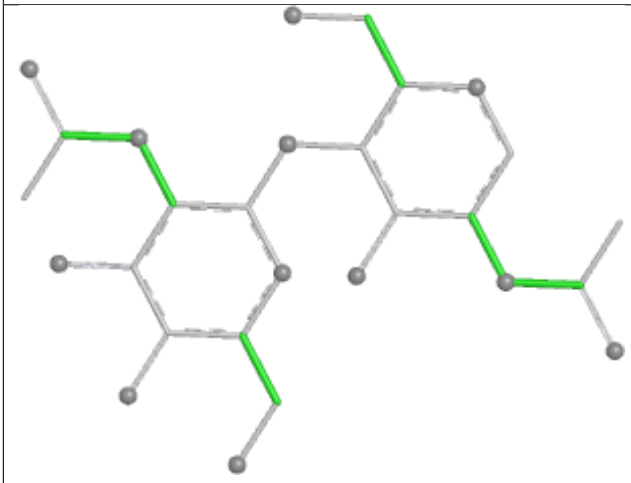
Oligosaccharide Chain J



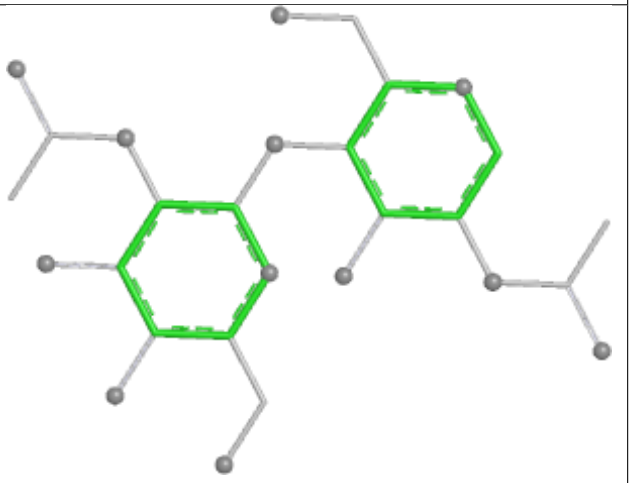
Bond lengths



Bond angles

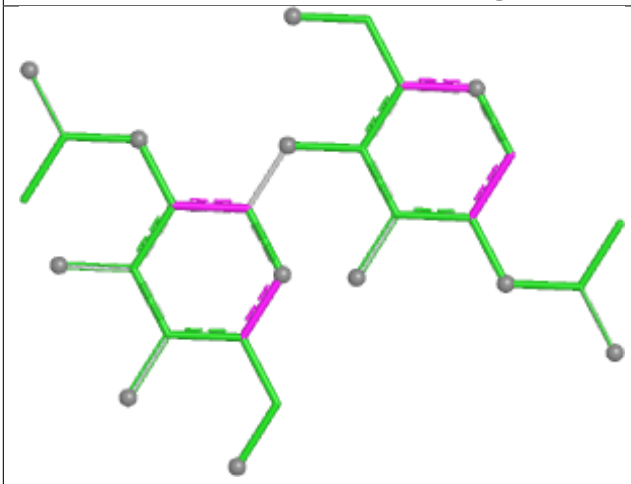


Torsions

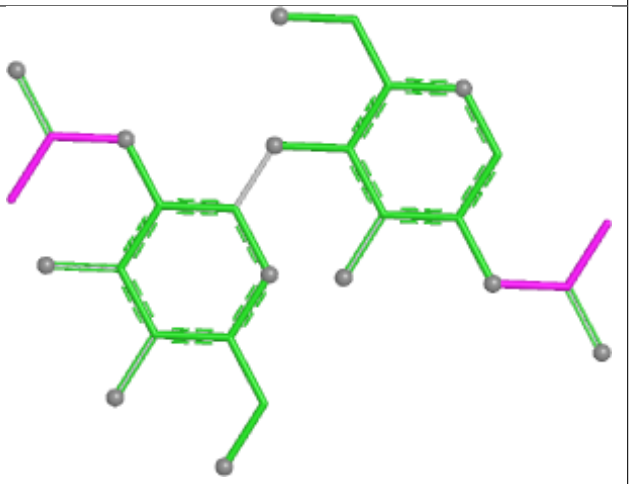


Rings

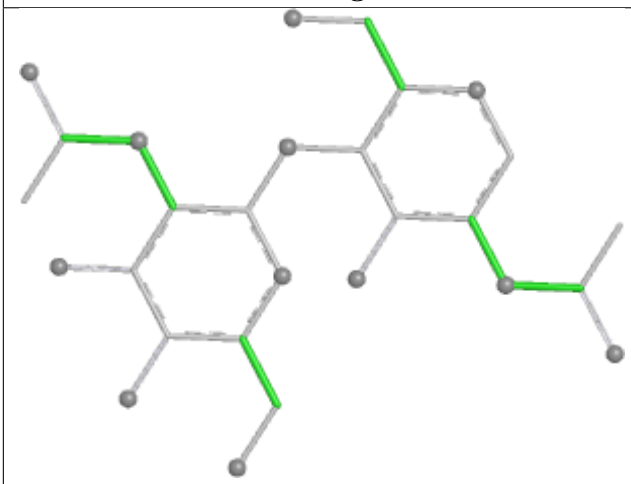
Oligosaccharide Chain M



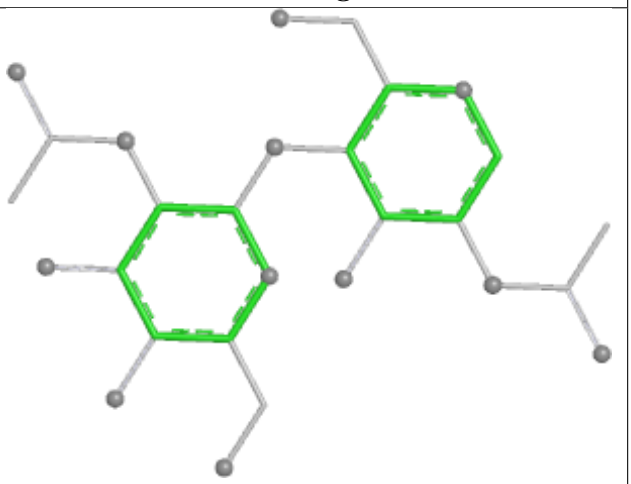
Bond lengths



Bond angles

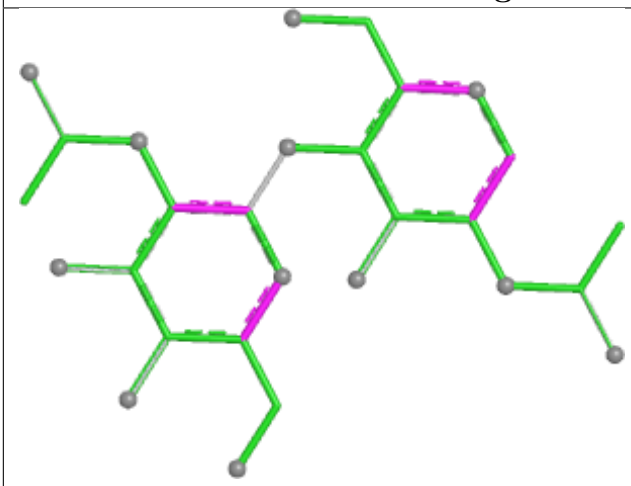


Torsions

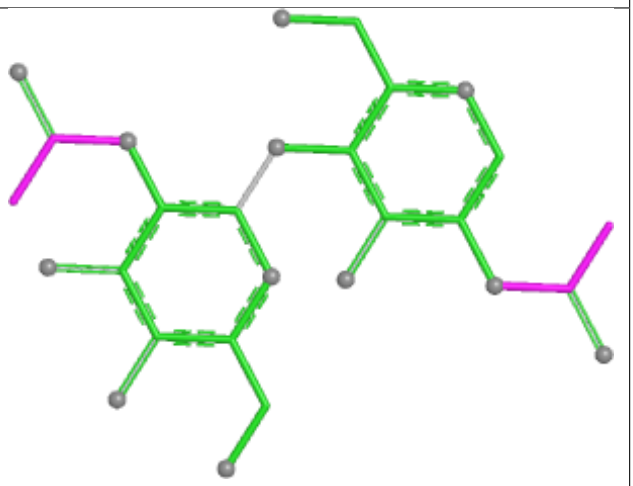


Rings

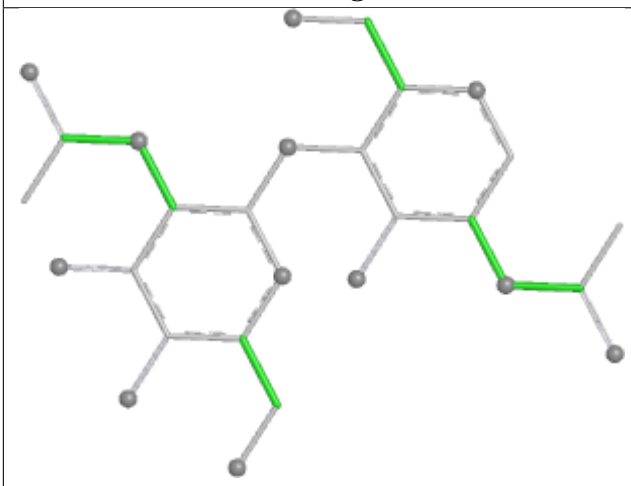
Oligosaccharide Chain O



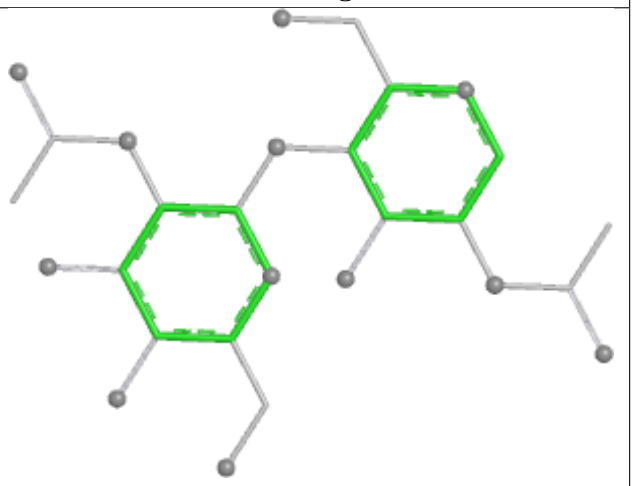
Bond lengths



Bond angles

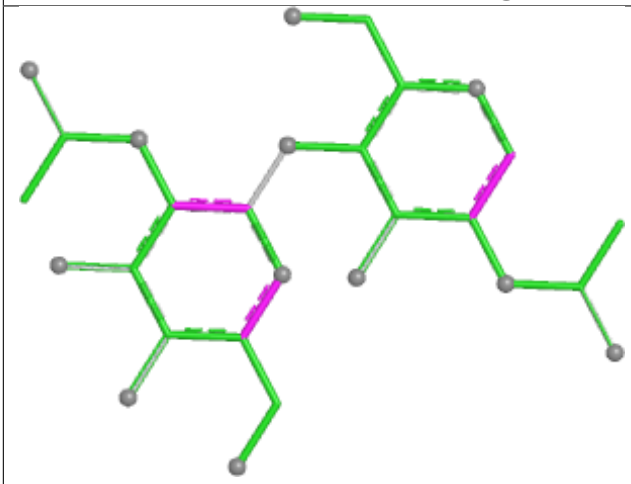


Torsions

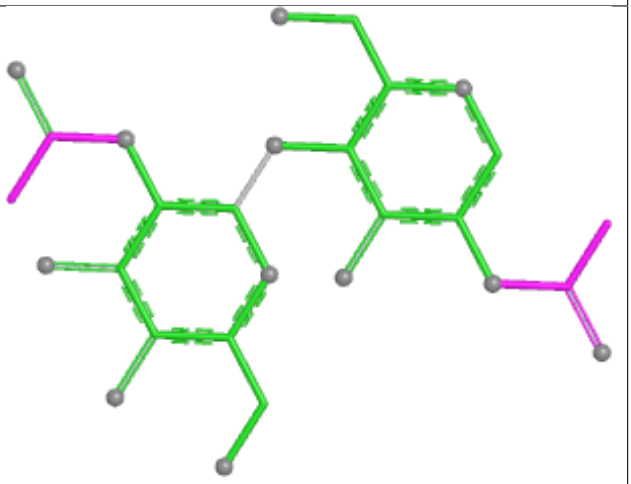


Rings

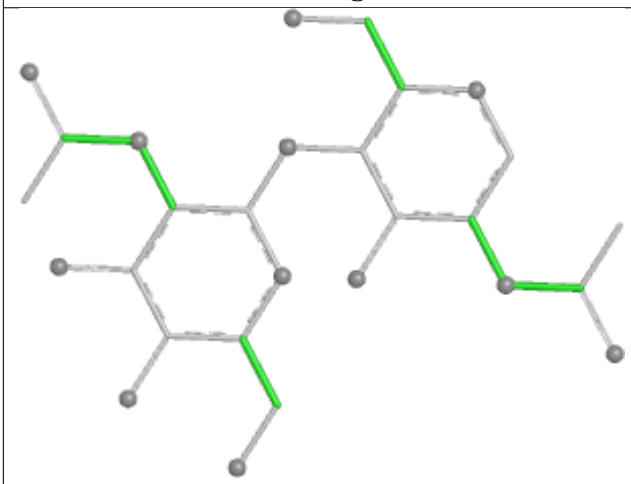
Oligosaccharide Chain S



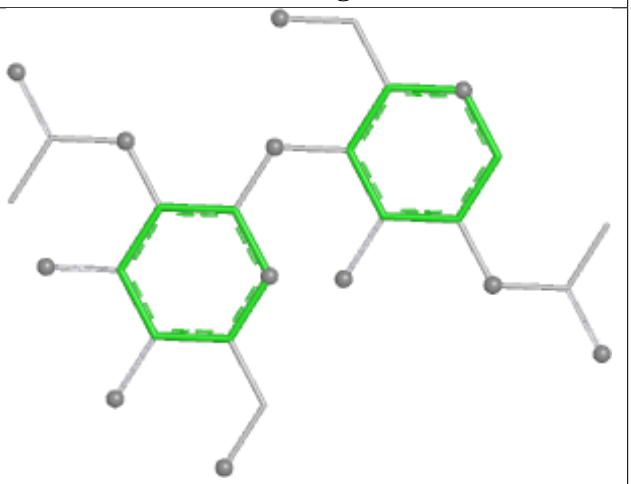
Bond lengths



Bond angles

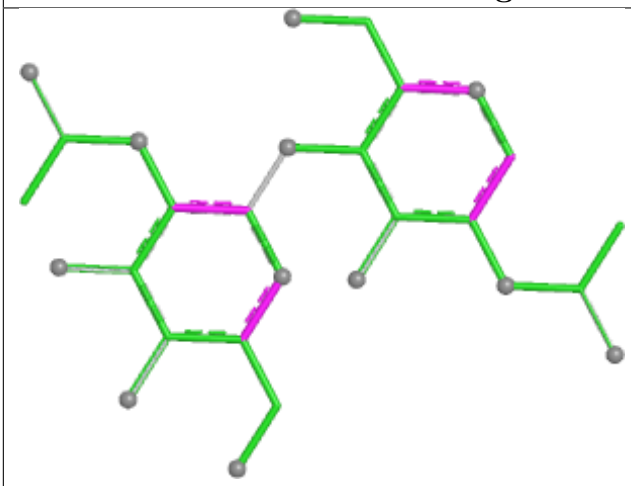


Torsions

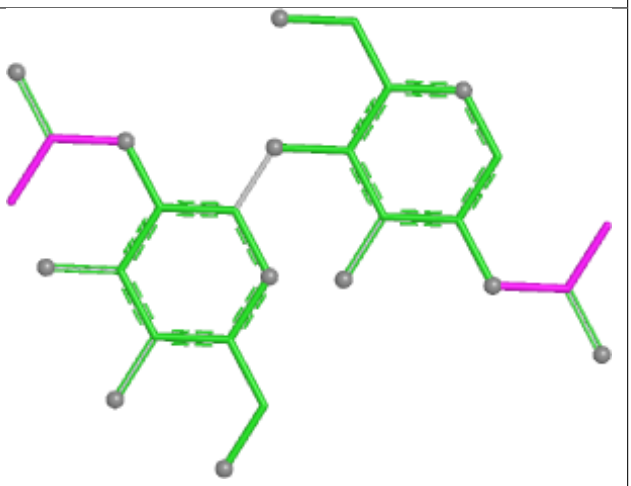


Rings

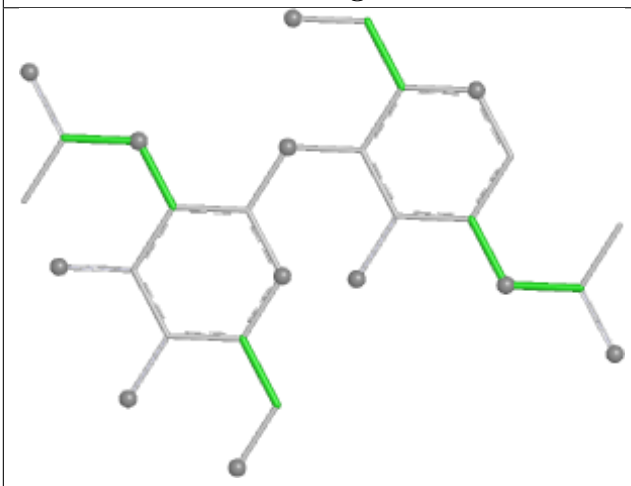
Oligosaccharide Chain T



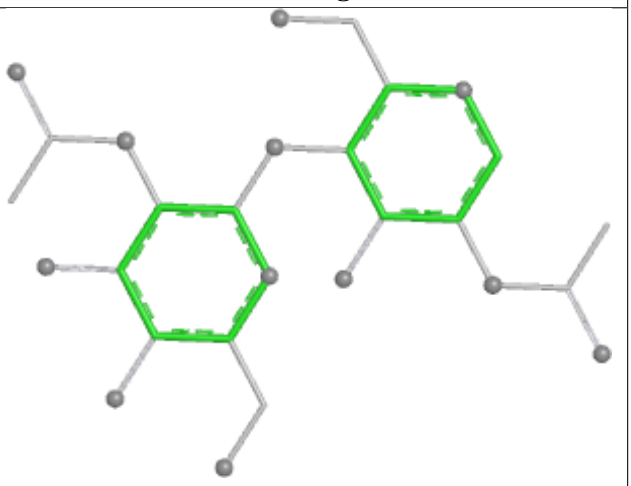
Bond lengths



Bond angles

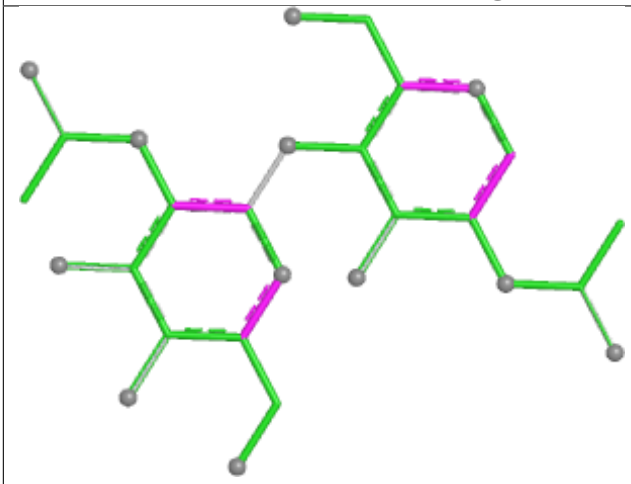


Torsions

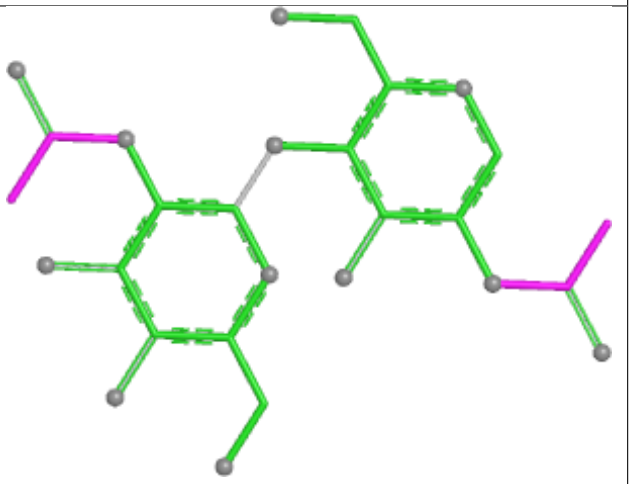


Rings

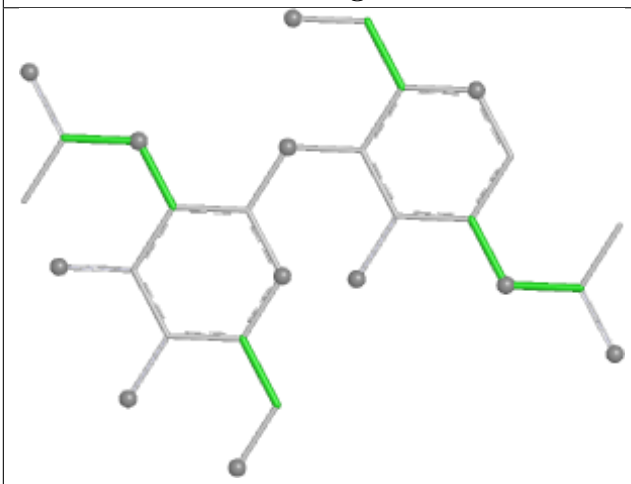
Oligosaccharide Chain W



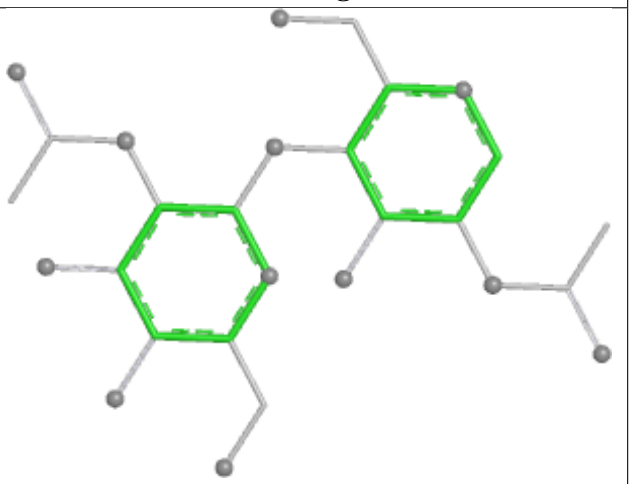
Bond lengths



Bond angles

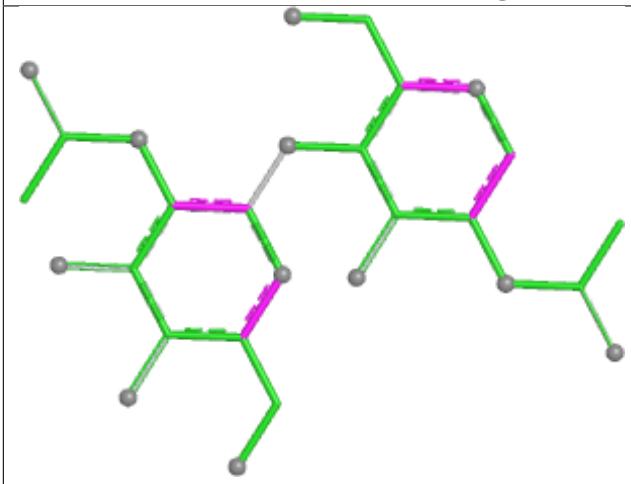


Torsions



Rings

Oligosaccharide Chain Y



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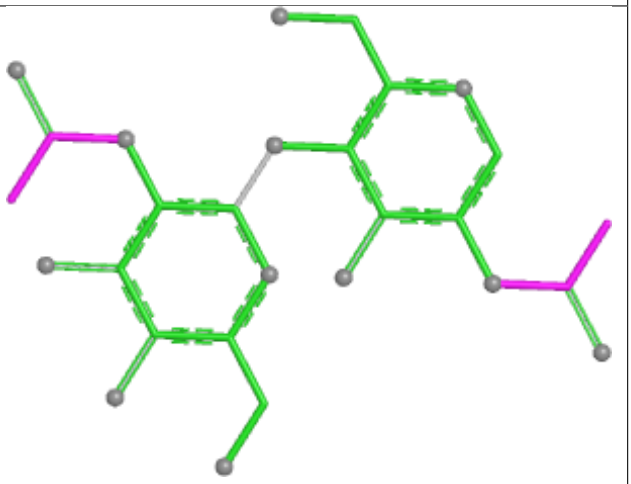
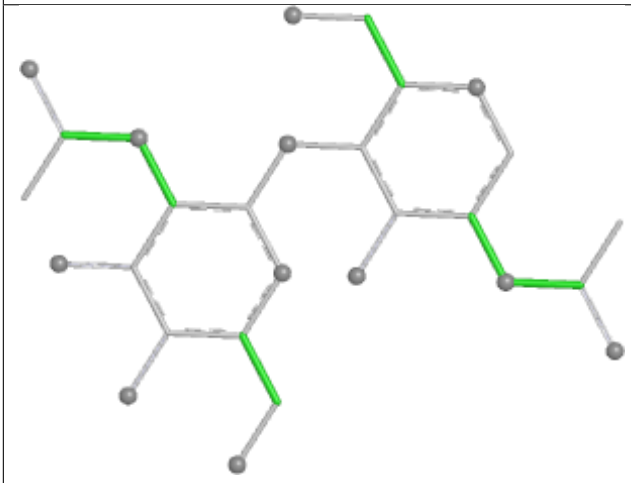


Bond angles



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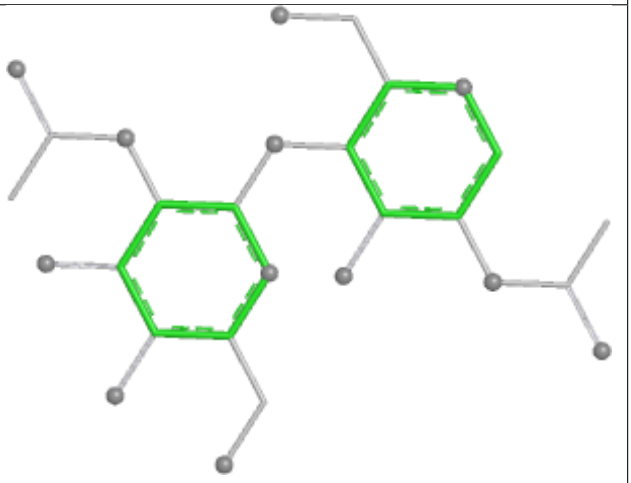
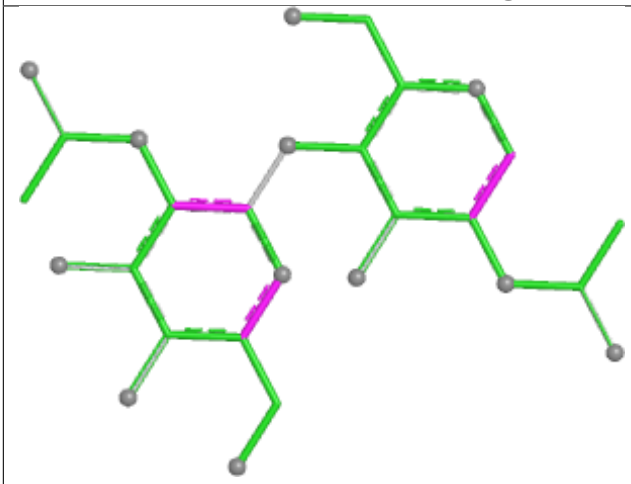


Rings

Oligosaccharide Chain c



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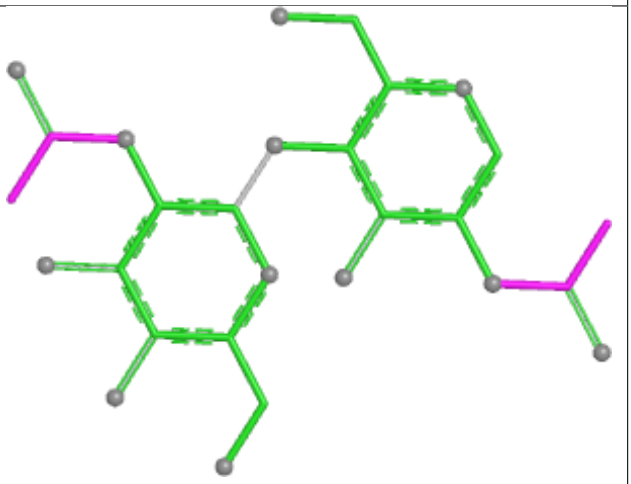
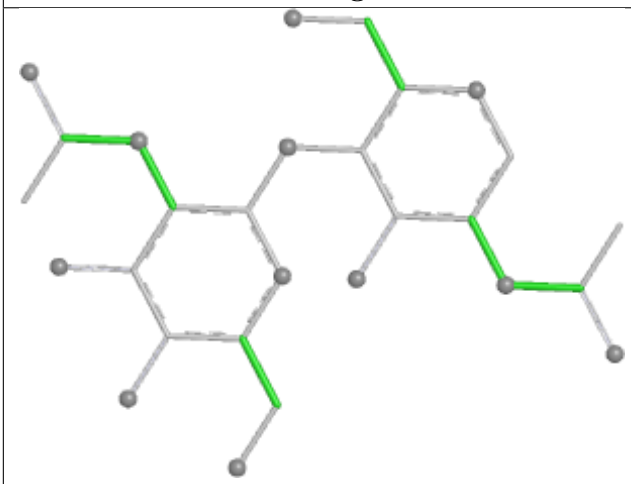


Bond angles



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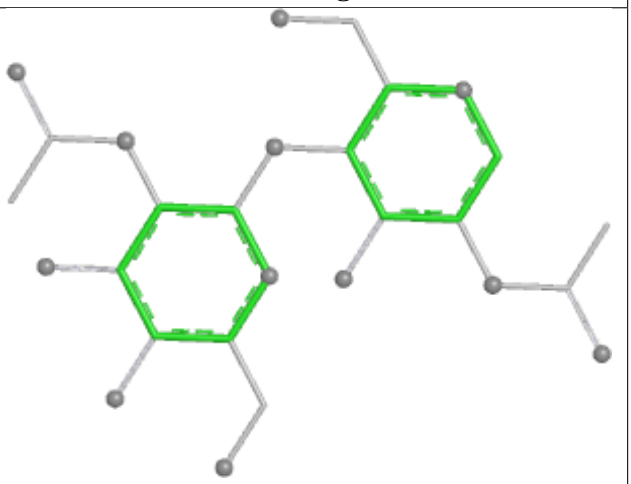
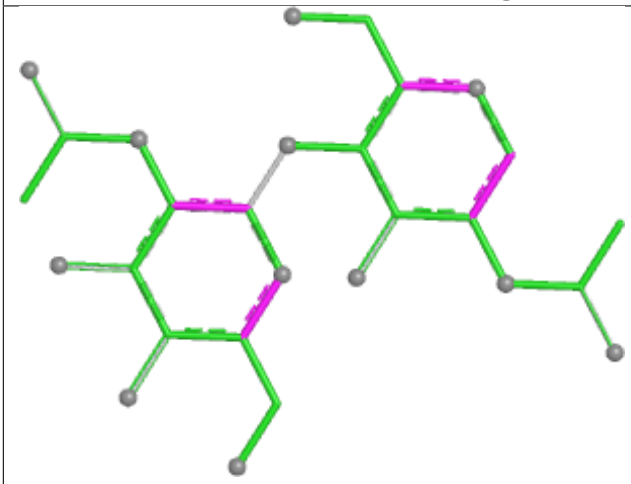


Rings

Oligosaccharide Chain d



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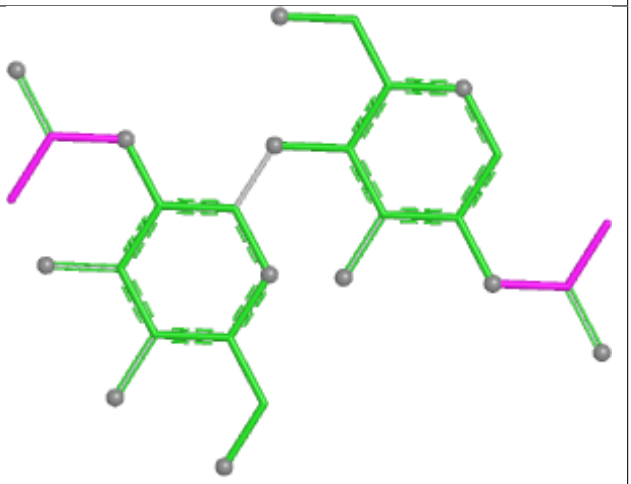

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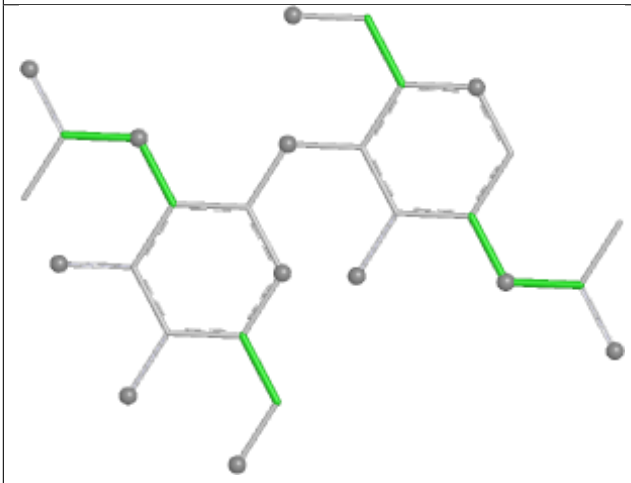
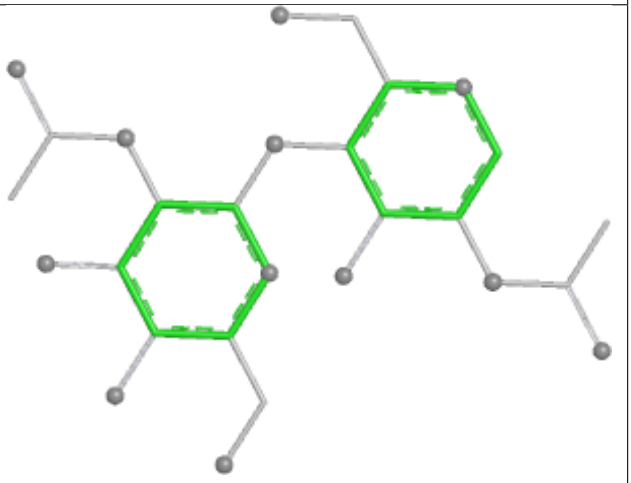
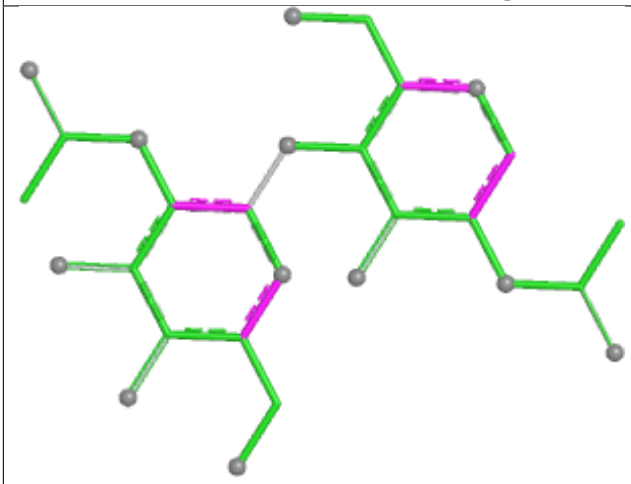


Torsions



Rings

Oligosaccharide Chain g



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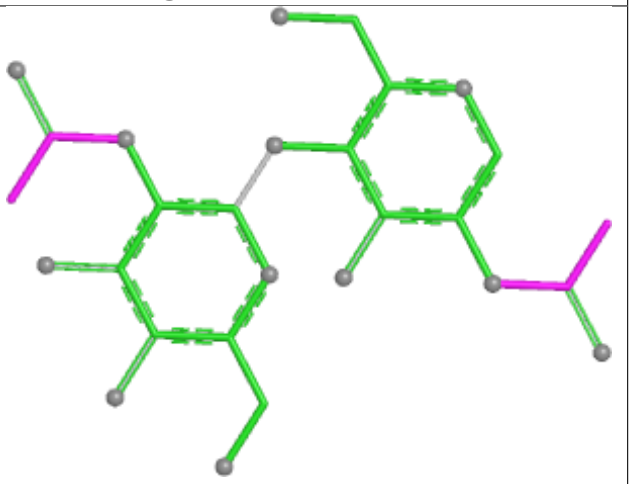
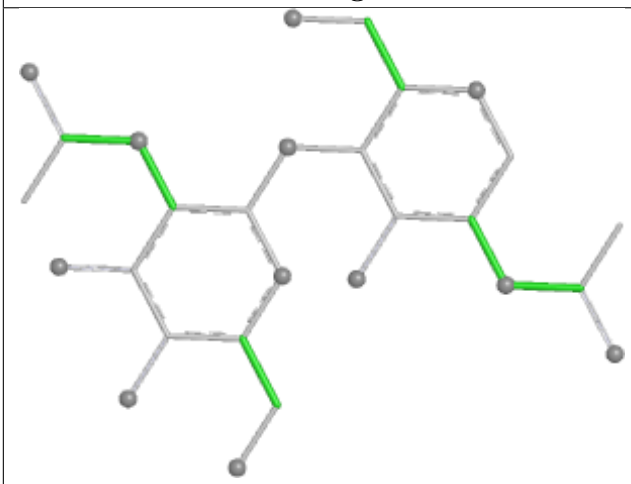


Bond angles



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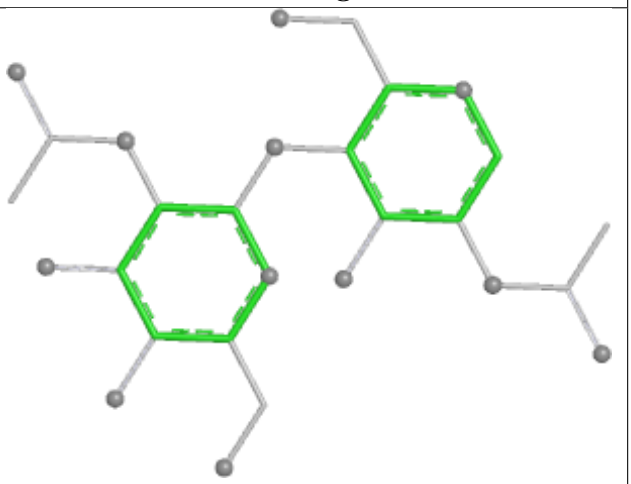
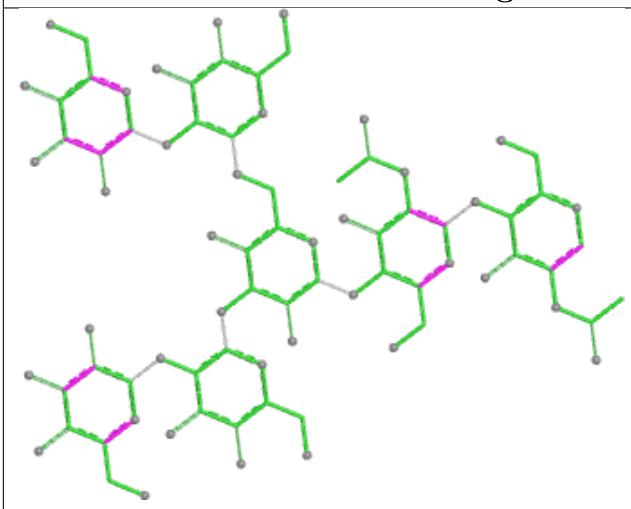


Rings

Oligosaccharide Chain F



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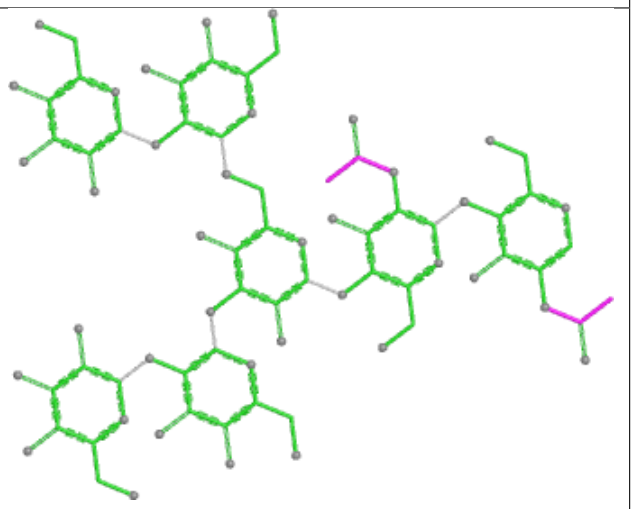
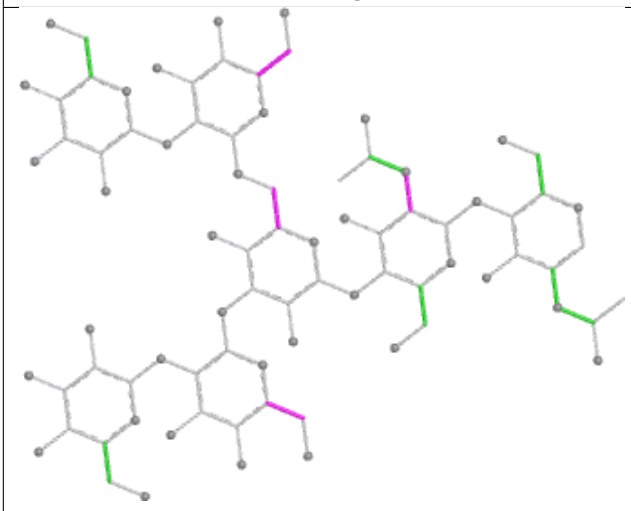


Bond angles



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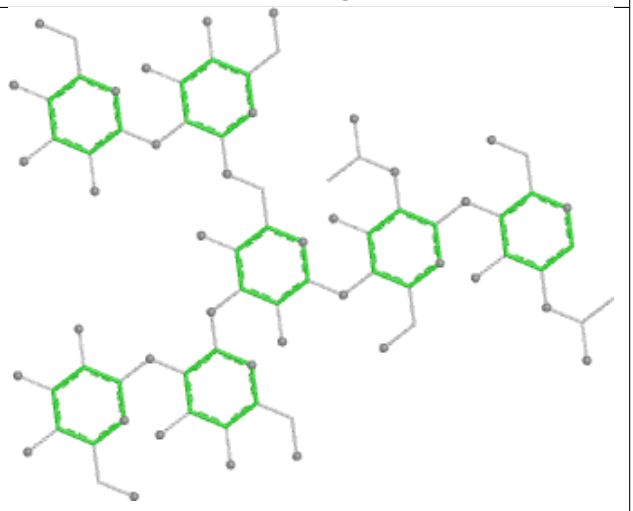
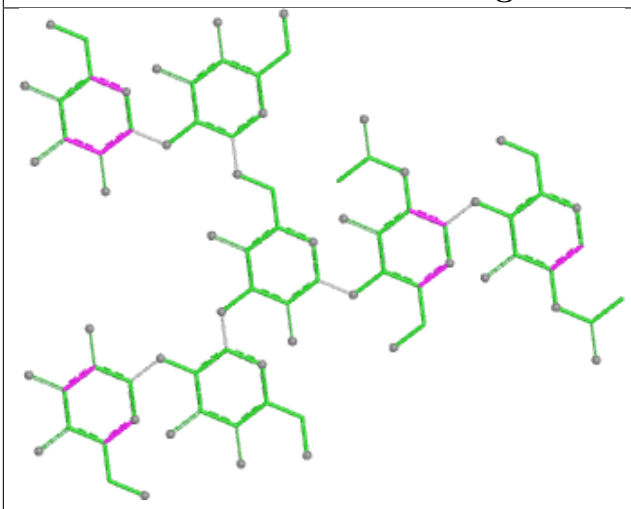


Rings

Oligosaccharide Chain P



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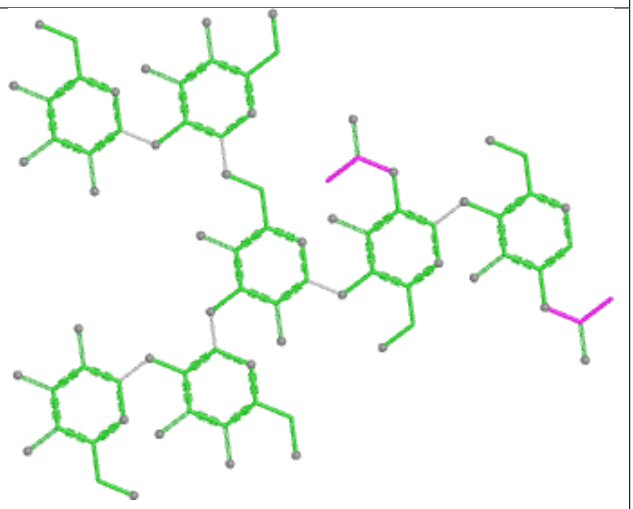
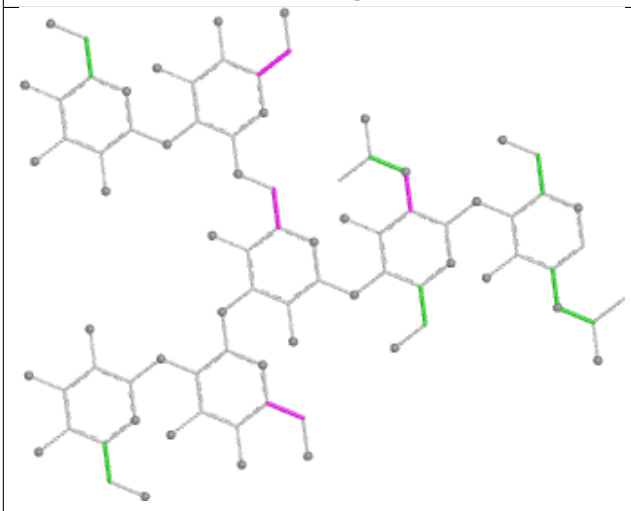


Bond angles



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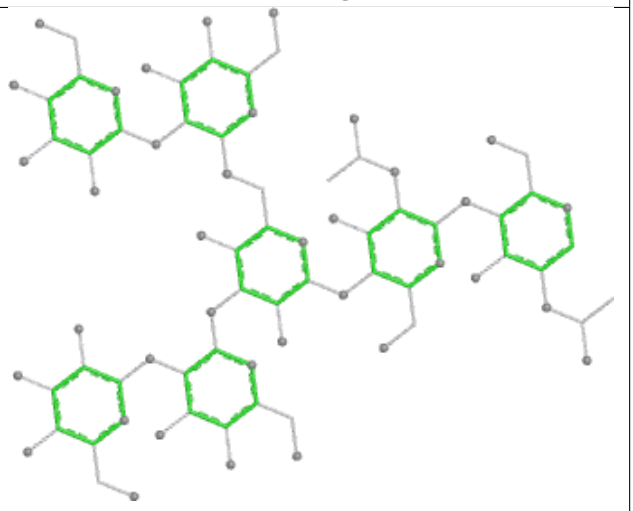
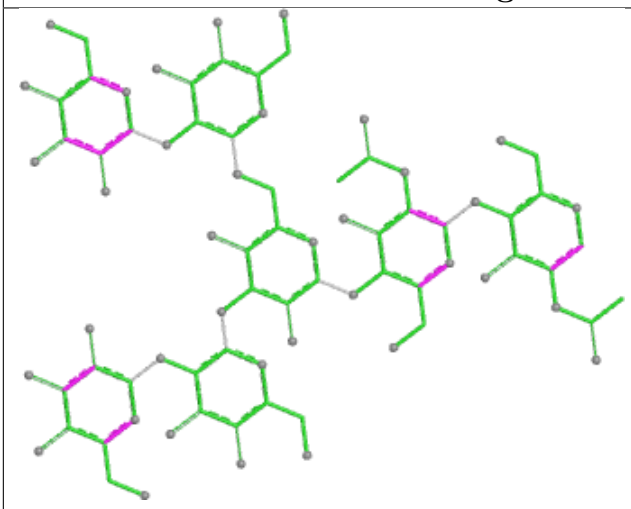


Rings

Oligosaccharide Chain Z



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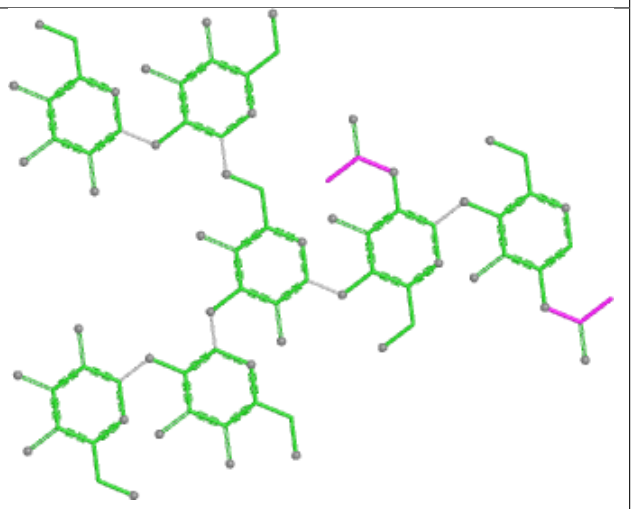
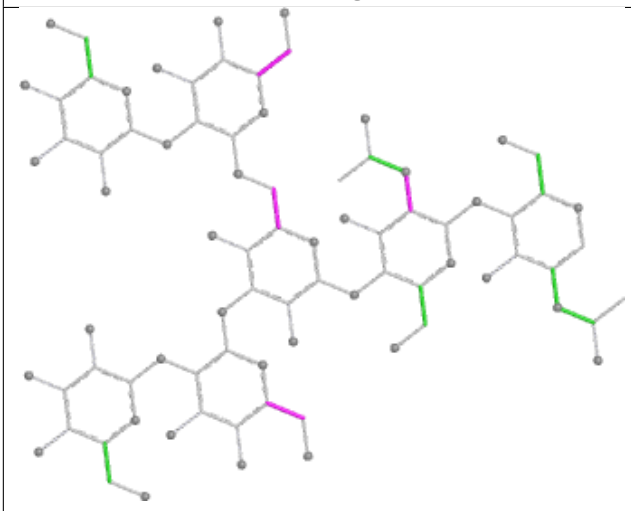


Bond angles



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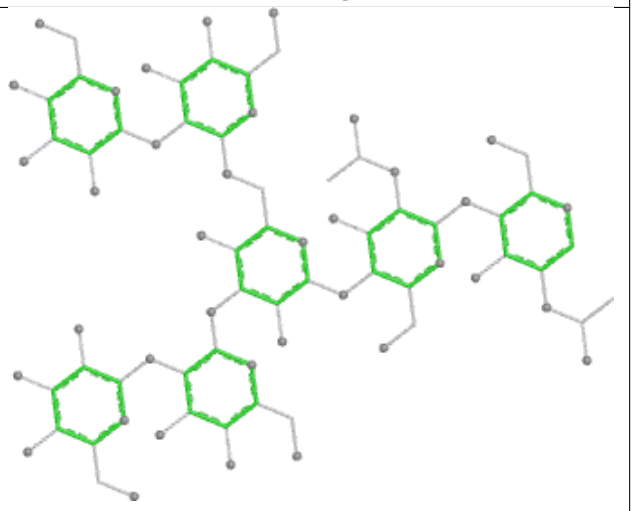
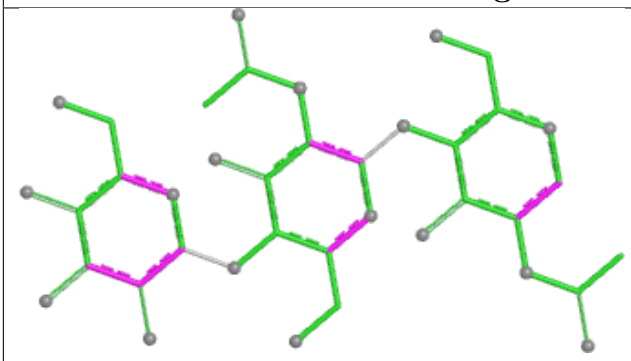


Rings

Oligosaccharide Chain G



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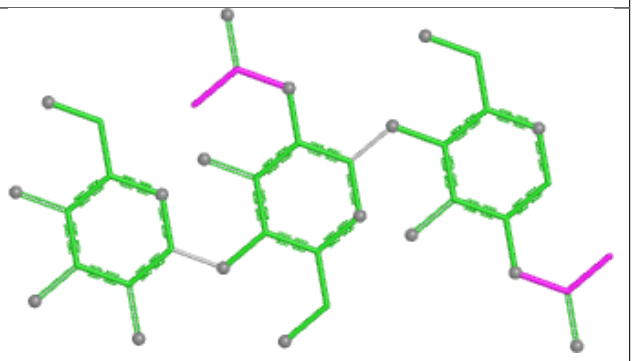
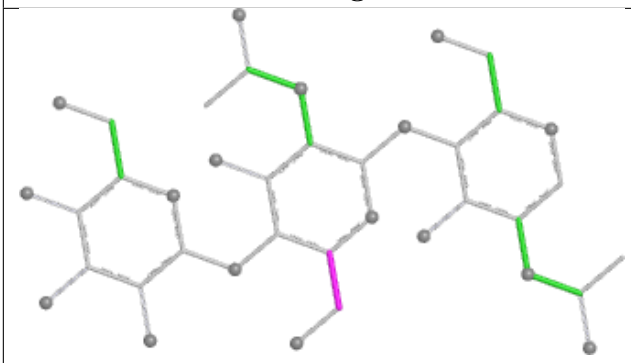


Bond angles



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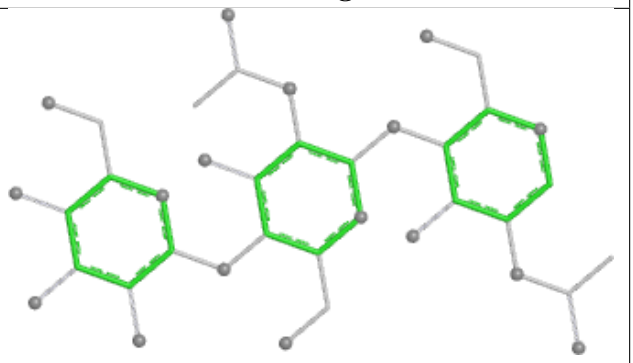
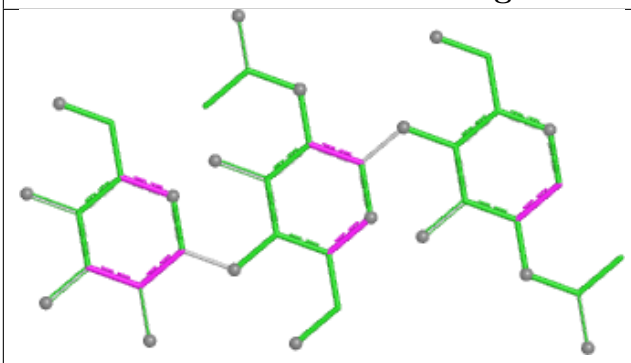


Rings

Oligosaccharide Chain Q



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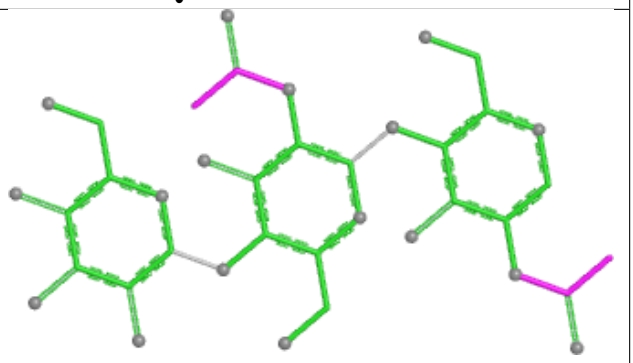
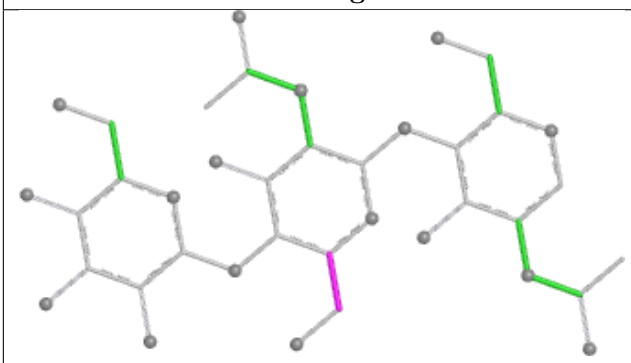


Bond angles



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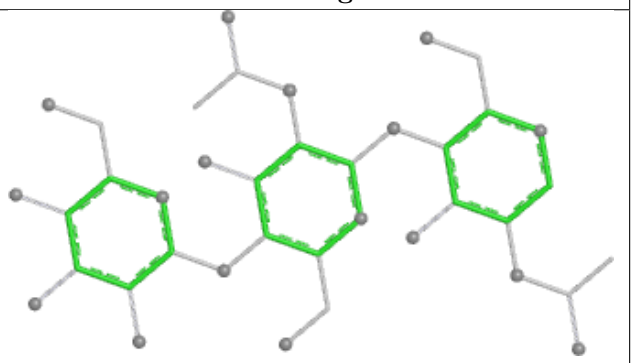
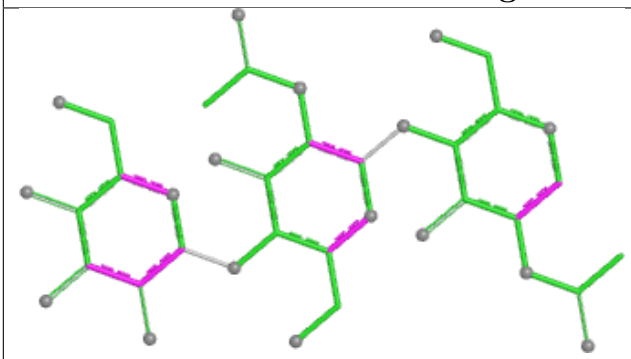


Rings

Oligosaccharide Chain a



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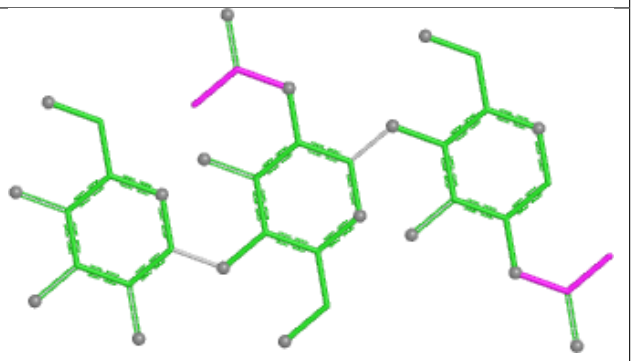
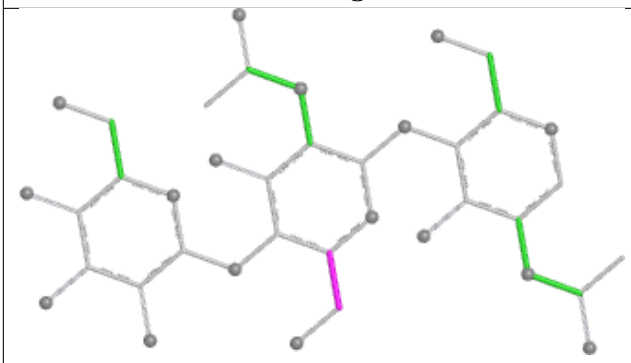


Bond angles



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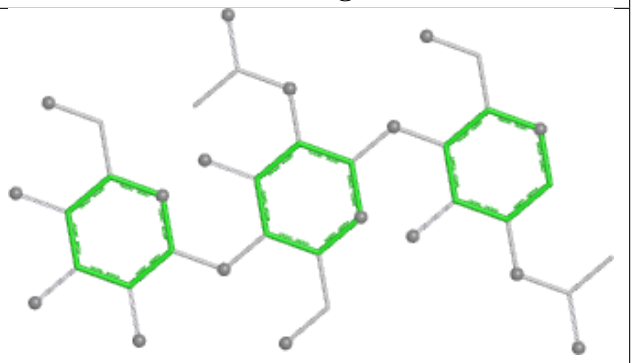
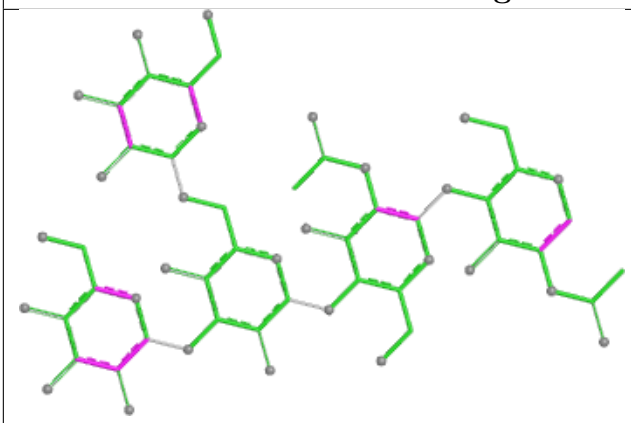


Rings

Oligosaccharide Chain K



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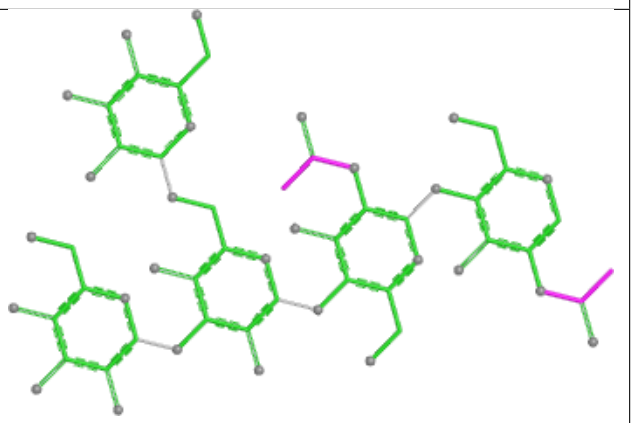
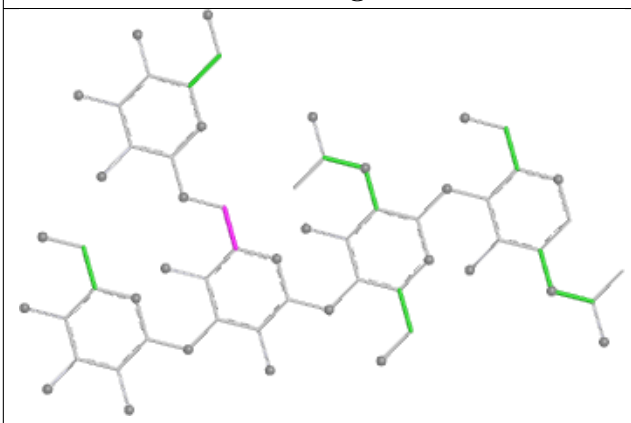


Bond angles



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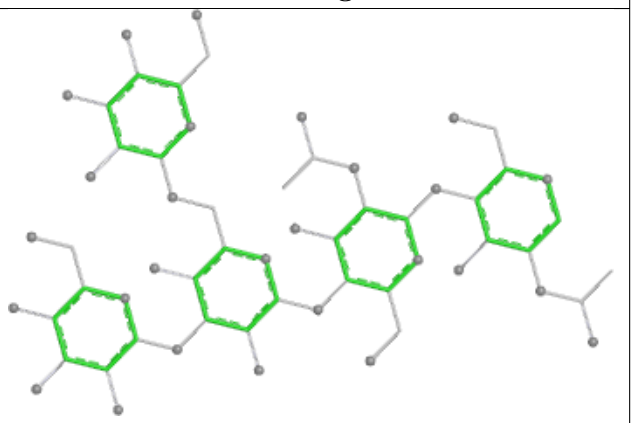
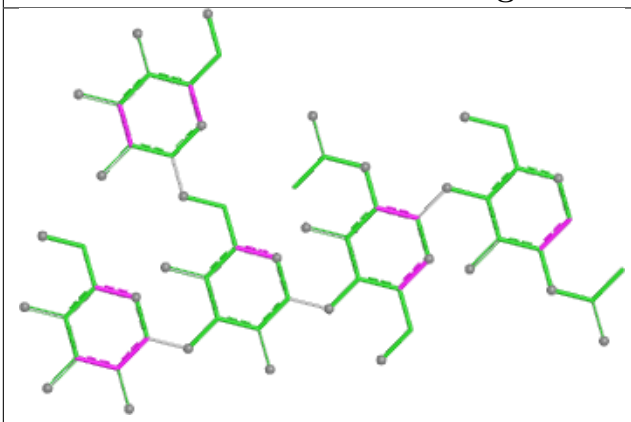


Rings

Oligosaccharide Chain L



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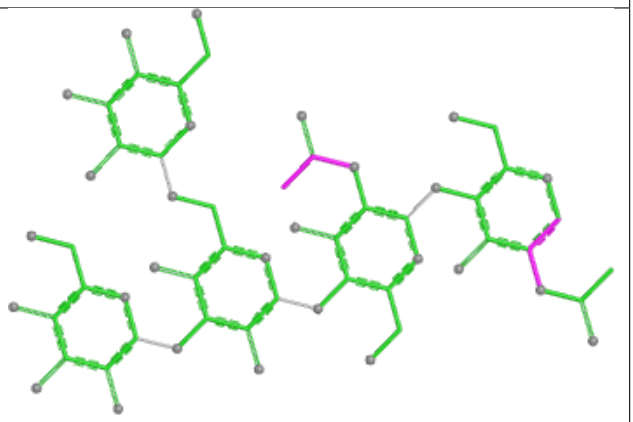
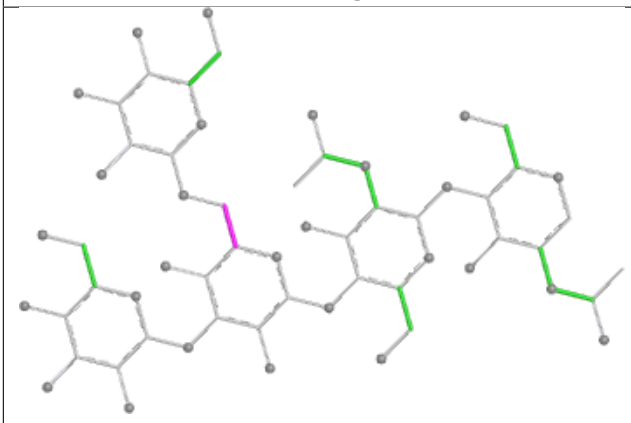
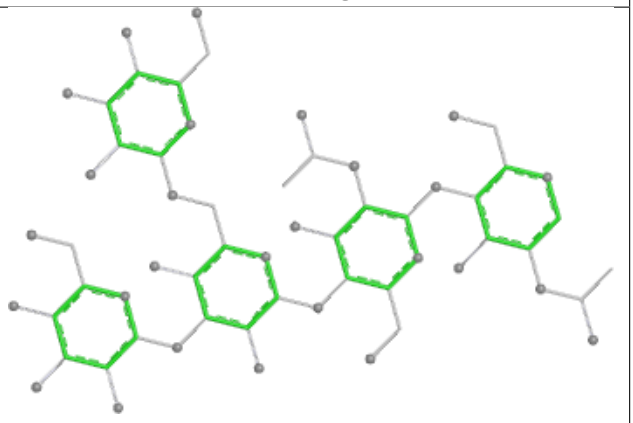


Bond angles

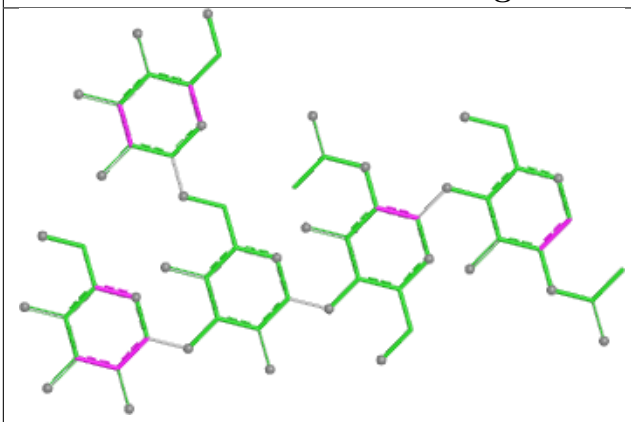


Torsions



Rings

Oligosaccharide Chain U



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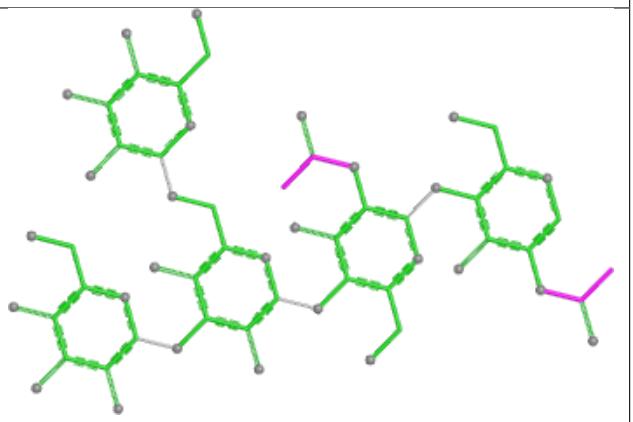
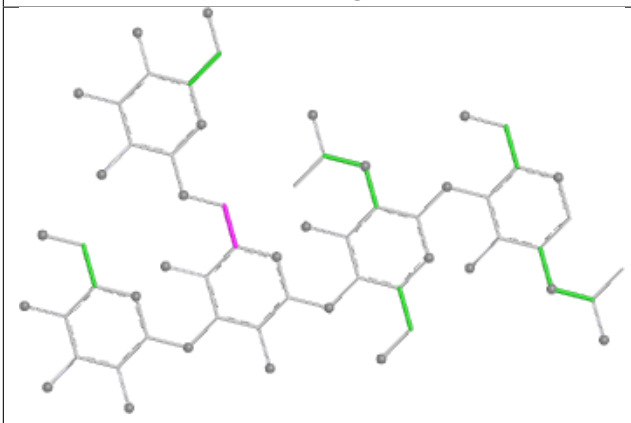


Bond angles



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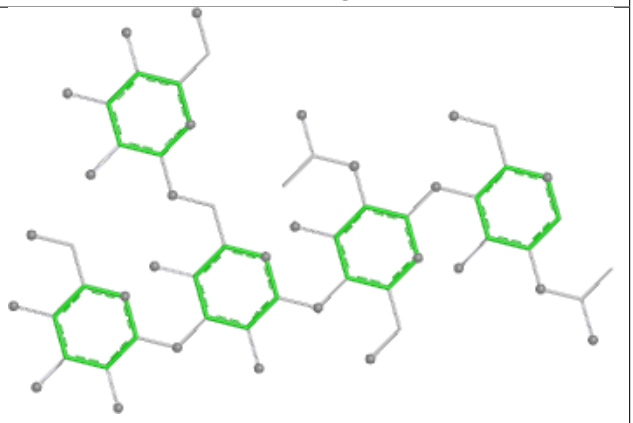
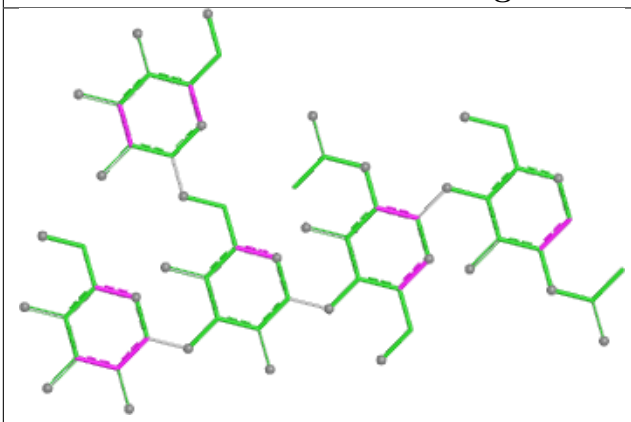
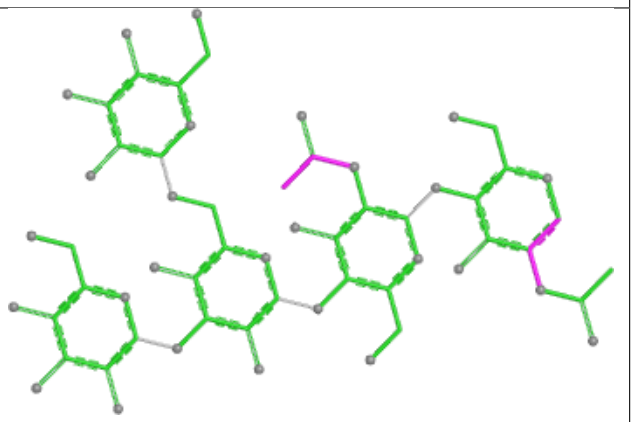


Rings

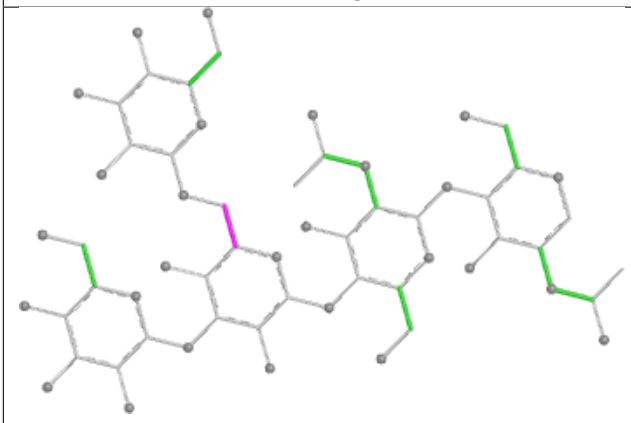
Oligosaccharide Chain V



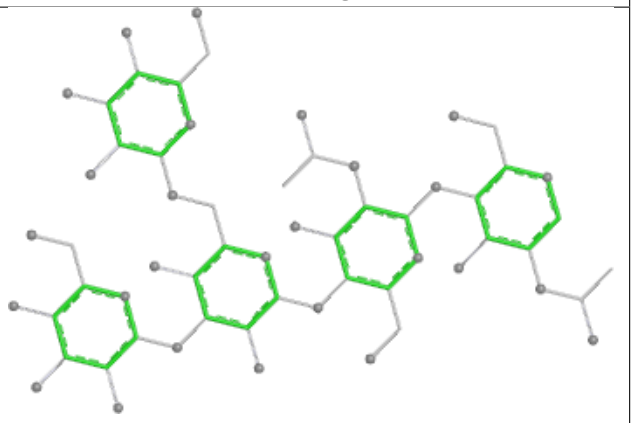
Bond lengths



Bond angles

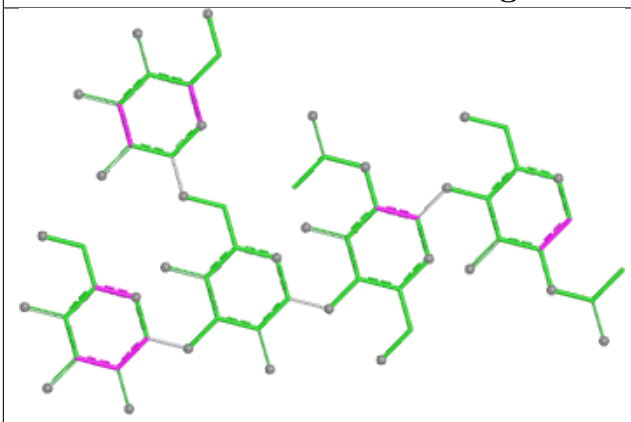


Torsions

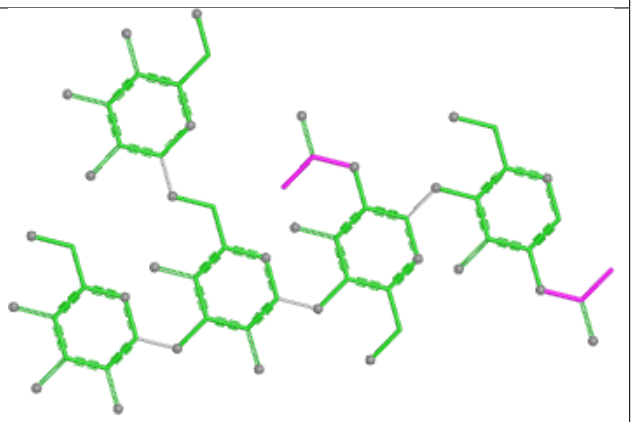


Rings

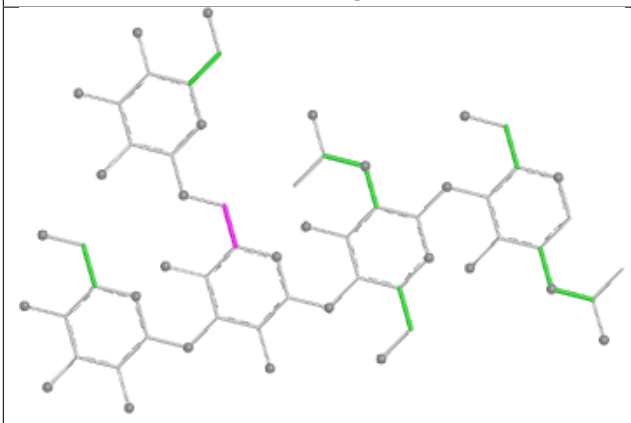
Oligosaccharide Chain e



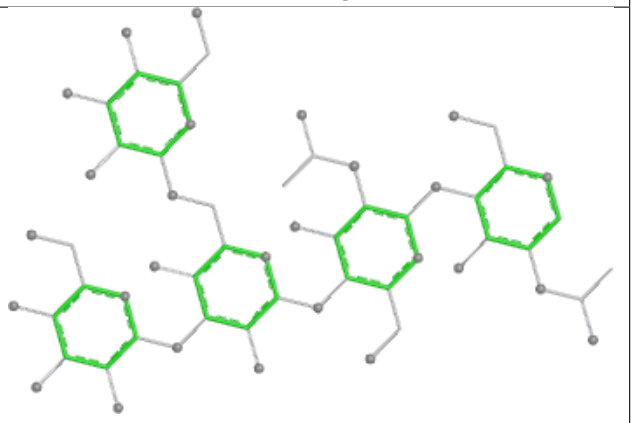
Bond lengths



Bond angles

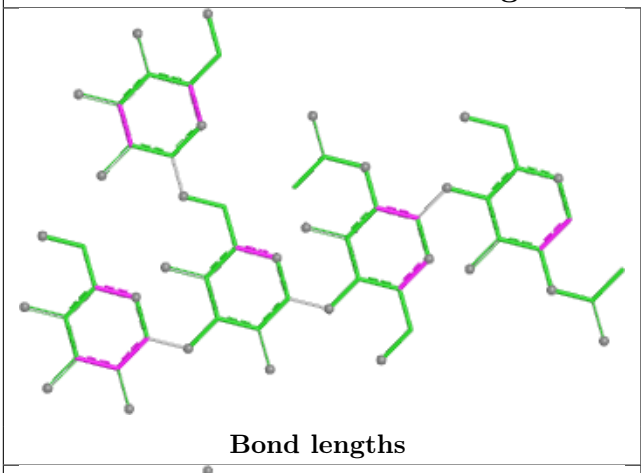


Torsions

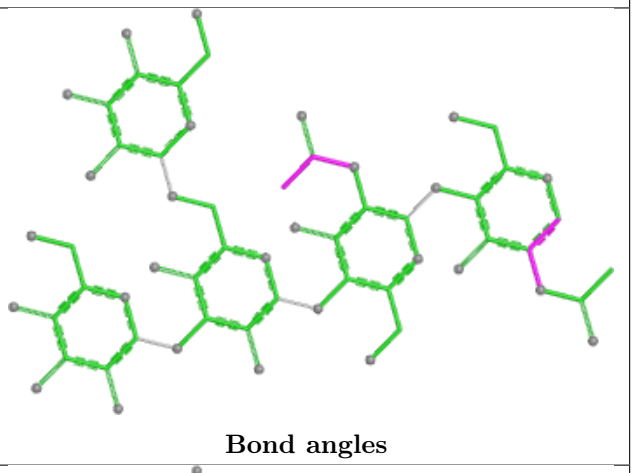


Rings

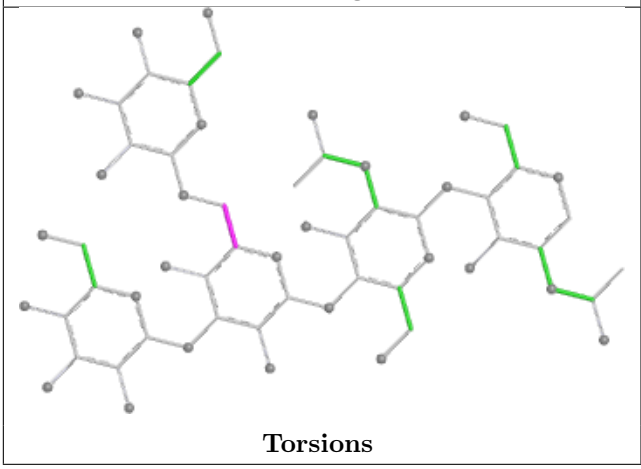
Oligosaccharide Chain f



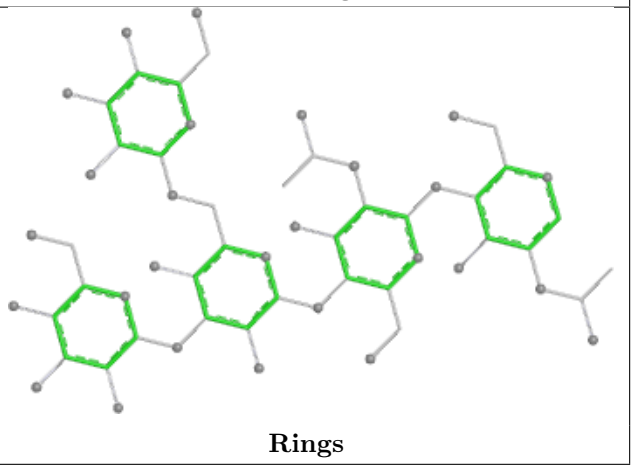
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

27 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	$\#\|Z\| > 2$
8	NAG	C	1402	1	14,14,15	1.63	2 (14%)	17,19,21	0.88	1 (5%)
8	NAG	E	1408	1	14,14,15	1.61	2 (14%)	17,19,21	1.05	1 (5%)
8	NAG	A	1408	1	14,14,15	1.62	2 (14%)	17,19,21	1.05	1 (5%)
8	NAG	C	1404	1	14,14,15	1.64	2 (14%)	17,19,21	0.92	1 (5%)
7	FOL	E	1401	-	34,34,34	1.32	3 (8%)	43,47,47	2.11	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	C	1408	1	14,14,15	1.62	2 (14%)	17,19,21	1.05	1 (5%)
8	NAG	E	1406	1	14,14,15	1.64	2 (14%)	17,19,21	1.00	1 (5%)
8	NAG	C	1403	1	14,14,15	1.62	2 (14%)	17,19,21	0.95	1 (5%)
7	FOL	C	1401	-	34,34,34	1.31	3 (8%)	43,47,47	2.11	8 (18%)
8	NAG	E	1403	1	14,14,15	1.63	2 (14%)	17,19,21	0.95	1 (5%)
8	NAG	E	1404	1	14,14,15	1.64	2 (14%)	17,19,21	0.92	1 (5%)
8	NAG	A	1402	1	14,14,15	1.63	2 (14%)	17,19,21	0.88	1 (5%)
8	NAG	C	1405	1	14,14,15	1.59	2 (14%)	17,19,21	1.01	1 (5%)
8	NAG	E	1402	1	14,14,15	1.64	2 (14%)	17,19,21	0.89	1 (5%)
9	SIA	C	1409	-	21,21,21	2.21	6 (28%)	24,31,31	1.26	2 (8%)
8	NAG	A	1405	1	14,14,15	1.59	2 (14%)	17,19,21	1.01	1 (5%)
8	NAG	A	1404	1	14,14,15	1.64	2 (14%)	17,19,21	0.92	1 (5%)
8	NAG	C	1406	1	14,14,15	1.65	2 (14%)	17,19,21	1.00	1 (5%)
9	SIA	A	1409	-	21,21,21	2.21	6 (28%)	24,31,31	1.25	2 (8%)
8	NAG	A	1403	1	14,14,15	1.63	2 (14%)	17,19,21	0.95	1 (5%)
8	NAG	C	1407	1	14,14,15	1.53	2 (14%)	17,19,21	1.00	1 (5%)
8	NAG	E	1405	1	14,14,15	1.59	2 (14%)	17,19,21	1.02	1 (5%)
8	NAG	A	1407	1	14,14,15	1.52	2 (14%)	17,19,21	0.99	1 (5%)
8	NAG	E	1407	1	14,14,15	1.53	2 (14%)	17,19,21	0.99	1 (5%)
9	SIA	E	1409	-	21,21,21	2.21	6 (28%)	24,31,31	1.25	2 (8%)
7	FOL	A	1401	-	34,34,34	1.32	3 (8%)	43,47,47	2.11	8 (18%)
8	NAG	A	1406	1	14,14,15	1.64	2 (14%)	17,19,21	1.00	1 (5%)

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
8	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1408	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
7	FOL	E	1401	-	-	2/22/22/22	0/3/3/3
8	NAG	C	1408	1	-	1/6/23/26	0/1/1/1
8	NAG	E	1406	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1403	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FOL	C	1401	-	-	2/22/22/22	0/3/3/3
8	NAG	E	1403	1	-	1/6/23/26	0/1/1/1
8	NAG	E	1404	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1402	1	-	0/6/23/26	0/1/1/1
9	SIA	C	1409	-	-	3/20/38/38	0/1/1/1
8	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
9	SIA	A	1409	-	-	3/20/38/38	0/1/1/1
8	NAG	A	1403	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1405	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1407	1	-	0/6/23/26	0/1/1/1
9	SIA	E	1409	-	-	3/20/38/38	0/1/1/1
7	FOL	A	1401	-	-	2/22/22/22	0/3/3/3
8	NAG	A	1406	1	-	0/6/23/26	0/1/1/1

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1409	SIA	C6-C5	5.74	1.62	1.53
9	E	1409	SIA	C6-C5	5.72	1.62	1.53
9	C	1409	SIA	C6-C5	5.68	1.62	1.53
9	E	1409	SIA	C3-C2	5.02	1.58	1.51
9	C	1409	SIA	C3-C2	5.00	1.58	1.51
9	A	1409	SIA	C3-C2	4.99	1.58	1.51
8	E	1402	NAG	C1-C2	4.70	1.58	1.52
8	A	1404	NAG	C1-C2	4.69	1.58	1.52
8	E	1404	NAG	C1-C2	4.67	1.58	1.52
8	C	1404	NAG	C1-C2	4.67	1.58	1.52
8	A	1402	NAG	C1-C2	4.63	1.58	1.52
8	C	1406	NAG	C1-C2	4.63	1.58	1.52
8	C	1402	NAG	C1-C2	4.63	1.58	1.52
8	A	1406	NAG	C1-C2	4.60	1.58	1.52
8	E	1406	NAG	C1-C2	4.59	1.58	1.52
8	C	1408	NAG	C1-C2	4.57	1.58	1.52
8	A	1408	NAG	C1-C2	4.56	1.58	1.52
8	E	1408	NAG	C1-C2	4.56	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1403	NAG	C1-C2	4.49	1.58	1.52
8	E	1403	NAG	C1-C2	4.49	1.58	1.52
8	C	1403	NAG	C1-C2	4.45	1.58	1.52
8	E	1405	NAG	C1-C2	4.34	1.58	1.52
8	A	1405	NAG	C1-C2	4.34	1.58	1.52
8	C	1405	NAG	C1-C2	4.33	1.58	1.52
8	C	1407	NAG	C1-C2	4.22	1.58	1.52
8	A	1407	NAG	C1-C2	4.17	1.58	1.52
8	E	1407	NAG	C1-C2	4.17	1.58	1.52
7	A	1401	FOL	C4A-C4	4.11	1.48	1.41
7	E	1401	FOL	C4A-C4	4.10	1.48	1.41
7	C	1401	FOL	C4A-C4	4.10	1.48	1.41
7	E	1401	FOL	C4A-C8A	4.08	1.48	1.40
7	A	1401	FOL	C4A-C8A	4.08	1.48	1.40
7	C	1401	FOL	C4A-C8A	4.07	1.48	1.40
9	C	1409	SIA	O2-C2	3.69	1.44	1.39
9	E	1409	SIA	O2-C2	3.68	1.44	1.39
9	A	1409	SIA	O2-C2	3.66	1.44	1.39
9	E	1409	SIA	O6-C2	-3.09	1.40	1.43
9	C	1409	SIA	O6-C2	-3.08	1.40	1.43
9	A	1409	SIA	O6-C2	-3.06	1.40	1.43
9	C	1409	SIA	C7-C6	2.65	1.56	1.52
9	E	1409	SIA	C7-C6	2.64	1.56	1.52
9	A	1409	SIA	C7-C6	2.63	1.56	1.52
8	E	1403	NAG	O5-C5	2.48	1.48	1.43
8	C	1404	NAG	O5-C5	2.47	1.48	1.43
8	C	1406	NAG	O5-C5	2.47	1.48	1.43
8	A	1404	NAG	O5-C5	2.46	1.48	1.43
8	E	1404	NAG	O5-C5	2.46	1.48	1.43
8	A	1403	NAG	O5-C5	2.45	1.48	1.43
8	C	1403	NAG	O5-C5	2.45	1.48	1.43
8	A	1406	NAG	O5-C5	2.45	1.48	1.43
8	E	1406	NAG	O5-C5	2.44	1.48	1.43
9	C	1409	SIA	O1A-C1	2.43	1.29	1.22
9	E	1409	SIA	O1A-C1	2.43	1.29	1.22
8	C	1405	NAG	O5-C5	2.42	1.48	1.43
8	C	1402	NAG	O5-C5	2.42	1.48	1.43
9	A	1409	SIA	O1A-C1	2.42	1.29	1.22
8	A	1402	NAG	O5-C5	2.42	1.48	1.43
8	E	1405	NAG	O5-C5	2.41	1.48	1.43
8	A	1405	NAG	O5-C5	2.41	1.48	1.43
8	E	1402	NAG	O5-C5	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	1407	NAG	O5-C5	2.34	1.48	1.43
8	A	1407	NAG	O5-C5	2.32	1.48	1.43
8	C	1407	NAG	O5-C5	2.28	1.47	1.43
8	C	1408	NAG	O5-C5	2.28	1.47	1.43
8	E	1408	NAG	O5-C5	2.26	1.47	1.43
8	A	1408	NAG	O5-C5	2.25	1.47	1.43
7	A	1401	FOL	C6-N5	2.07	1.35	1.32
7	C	1401	FOL	C6-N5	2.06	1.35	1.32
7	E	1401	FOL	C6-N5	2.05	1.35	1.32

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1401	FOL	C2-N1-C8A	5.94	121.88	115.48
7	A	1401	FOL	C2-N1-C8A	5.93	121.88	115.48
7	E	1401	FOL	C2-N1-C8A	5.91	121.85	115.48
7	C	1401	FOL	N8-C8A-N1	5.53	121.79	115.77
7	A	1401	FOL	N8-C8A-N1	5.52	121.78	115.77
7	E	1401	FOL	N8-C8A-N1	5.48	121.74	115.77
7	E	1401	FOL	C8A-C4A-C4	-5.10	116.80	119.96
7	C	1401	FOL	C8A-C4A-C4	-5.10	116.80	119.96
7	A	1401	FOL	C8A-C4A-C4	-5.08	116.81	119.96
7	A	1401	FOL	C2-N3-C4	4.48	122.19	115.96
7	E	1401	FOL	C2-N3-C4	4.47	122.17	115.96
7	C	1401	FOL	C2-N3-C4	4.46	122.16	115.96
7	A	1401	FOL	C4A-C4-N3	-4.33	117.63	123.42
7	E	1401	FOL	C4A-C4-N3	-4.31	117.66	123.42
7	C	1401	FOL	C4A-C4-N3	-4.30	117.67	123.42
7	A	1401	FOL	N1-C2-N3	-3.78	122.40	127.21
7	C	1401	FOL	N1-C2-N3	-3.78	122.41	127.21
7	E	1401	FOL	N1-C2-N3	-3.78	122.41	127.21
8	E	1405	NAG	C8-C7-N2	2.68	120.56	116.12
8	C	1405	NAG	C8-C7-N2	2.68	120.56	116.12
8	A	1405	NAG	C8-C7-N2	2.68	120.56	116.12
9	C	1409	SIA	C4-C5-N5	-2.53	105.46	110.44
9	A	1409	SIA	C4-C5-N5	-2.53	105.46	110.44
9	A	1409	SIA	O2-C2-C1	-2.53	105.39	110.73
9	C	1409	SIA	O2-C2-C1	-2.52	105.40	110.73
9	E	1409	SIA	O2-C2-C1	-2.52	105.41	110.73
9	E	1409	SIA	C4-C5-N5	-2.52	105.48	110.44
8	E	1408	NAG	C8-C7-N2	2.44	120.16	116.12
7	E	1401	FOL	C8A-C4A-N5	-2.43	119.71	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1408	NAG	C8-C7-N2	2.40	120.11	116.12
7	C	1401	FOL	C8A-C4A-N5	-2.40	119.74	122.30
8	C	1408	NAG	C8-C7-N2	2.40	120.09	116.12
7	A	1401	FOL	C8A-C4A-N5	-2.40	119.74	122.30
8	A	1404	NAG	C8-C7-N2	2.37	120.04	116.12
8	E	1404	NAG	C8-C7-N2	2.36	120.04	116.12
8	C	1404	NAG	C8-C7-N2	2.36	120.03	116.12
8	C	1403	NAG	C8-C7-N2	2.34	120.00	116.12
8	A	1403	NAG	C8-C7-N2	2.34	120.00	116.12
8	E	1403	NAG	C8-C7-N2	2.34	119.99	116.12
8	C	1407	NAG	C8-C7-N2	2.33	119.97	116.12
8	E	1407	NAG	C8-C7-N2	2.31	119.95	116.12
8	A	1407	NAG	C8-C7-N2	2.30	119.94	116.12
8	C	1406	NAG	C8-C7-N2	2.30	119.92	116.12
8	A	1406	NAG	C8-C7-N2	2.29	119.92	116.12
8	E	1406	NAG	C8-C7-N2	2.29	119.91	116.12
7	C	1401	FOL	C11-C-N	2.26	121.24	117.04
7	E	1401	FOL	C11-C-N	2.26	121.23	117.04
7	A	1401	FOL	C11-C-N	2.26	121.22	117.04
8	E	1402	NAG	C8-C7-N2	2.04	119.51	116.12
8	A	1402	NAG	C8-C7-N2	2.03	119.48	116.12
8	C	1402	NAG	C8-C7-N2	2.02	119.47	116.12

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1409	SIA	O8-C8-C9-O9
9	C	1409	SIA	O8-C8-C9-O9
9	E	1409	SIA	O8-C8-C9-O9
9	A	1409	SIA	C7-C8-C9-O9
9	C	1409	SIA	C7-C8-C9-O9
9	E	1409	SIA	C7-C8-C9-O9
8	A	1408	NAG	O5-C5-C6-O6
8	C	1408	NAG	O5-C5-C6-O6
8	E	1408	NAG	O5-C5-C6-O6
7	A	1401	FOL	OE1-CD-CG-CB
7	C	1401	FOL	OE1-CD-CG-CB
7	E	1401	FOL	OE1-CD-CG-CB
8	A	1403	NAG	C1-C2-N2-C7
8	C	1403	NAG	C1-C2-N2-C7
8	E	1403	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	1401	FOL	OE2-CD-CG-CB
7	A	1401	FOL	OE2-CD-CG-CB
7	E	1401	FOL	OE2-CD-CG-CB
9	A	1409	SIA	O1B-C1-C2-C3
9	C	1409	SIA	O1B-C1-C2-C3
9	E	1409	SIA	O1B-C1-C2-C3

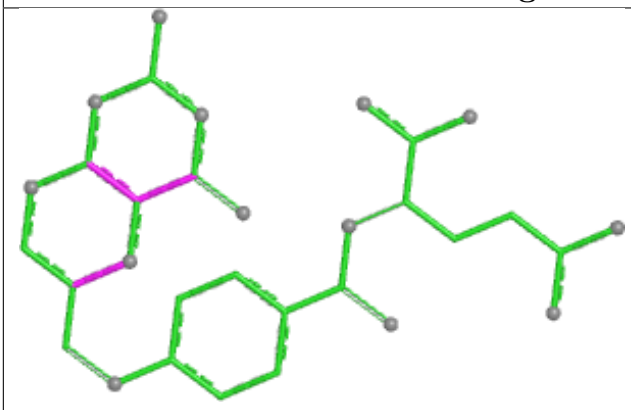
There are no ring outliers.

6 monomers are involved in 12 short contacts:

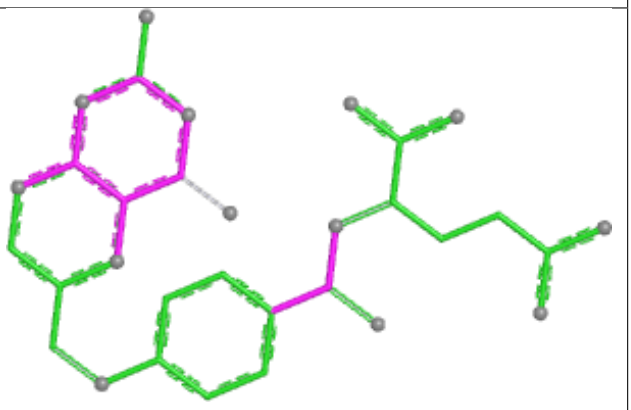
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1401	FOL	1	0
7	C	1401	FOL	1	0
9	C	1409	SIA	3	0
9	A	1409	SIA	3	0
9	E	1409	SIA	3	0
7	A	1401	FOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

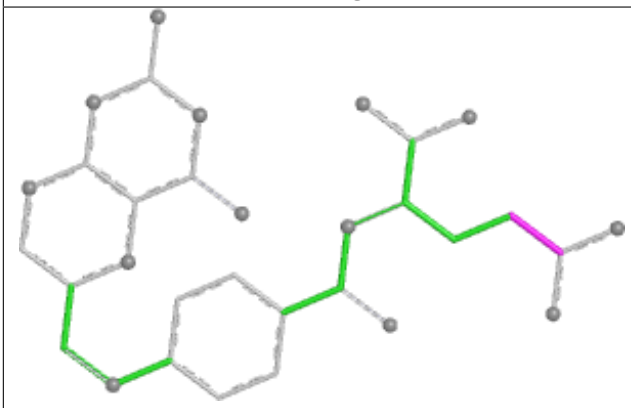
Ligand FOL E 1401



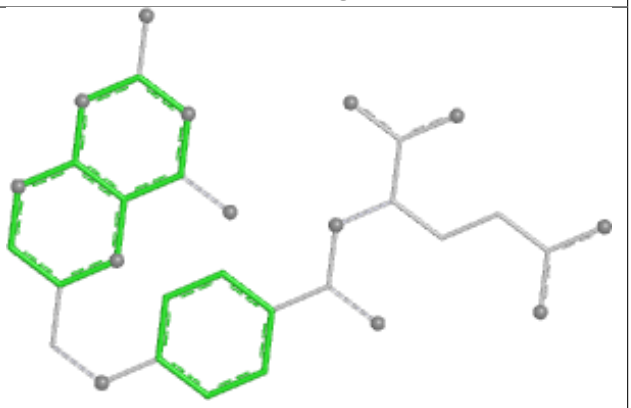
Bond lengths



Bond angles

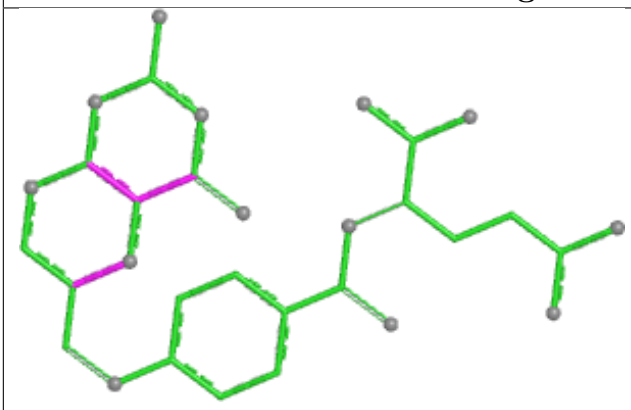


Torsions

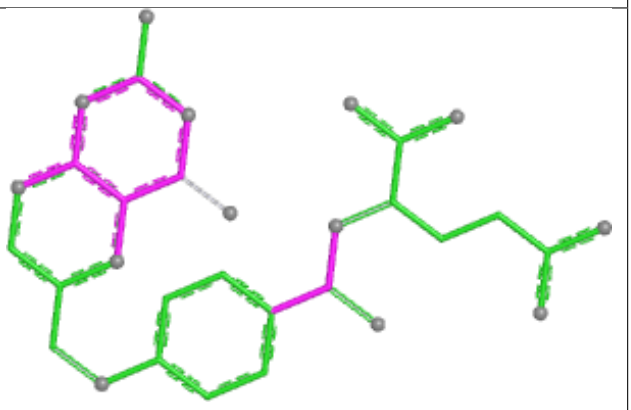


Rings

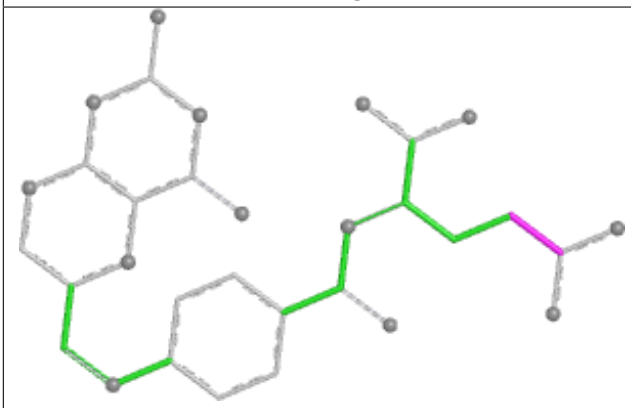
Ligand FOL C 1401



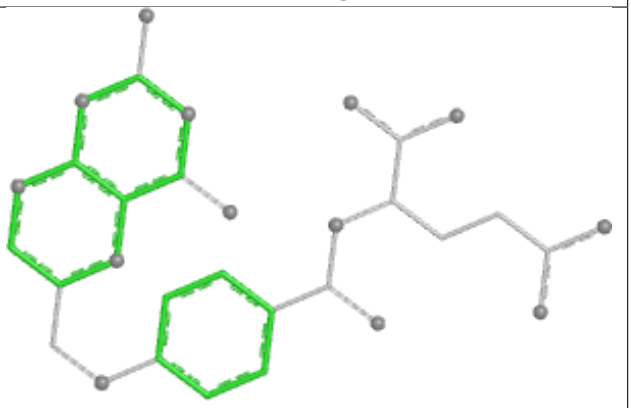
Bond lengths



Bond angles

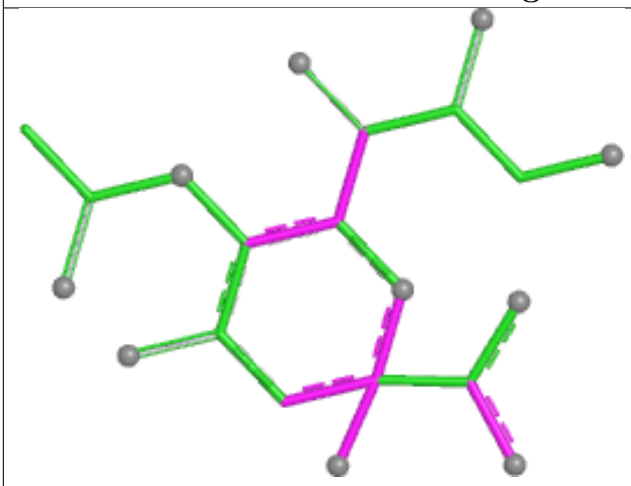


Torsions

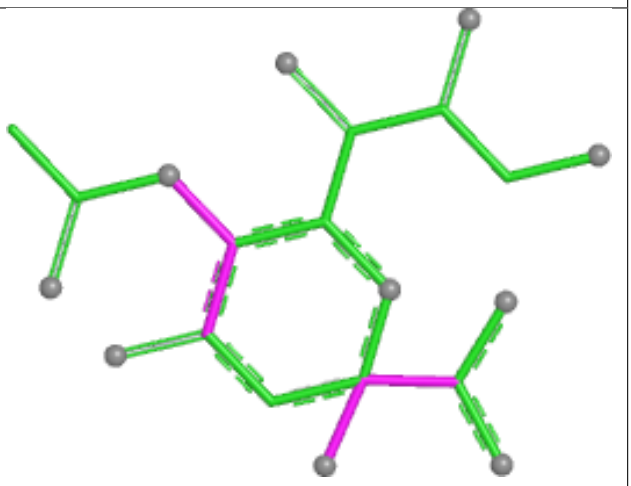


Rings

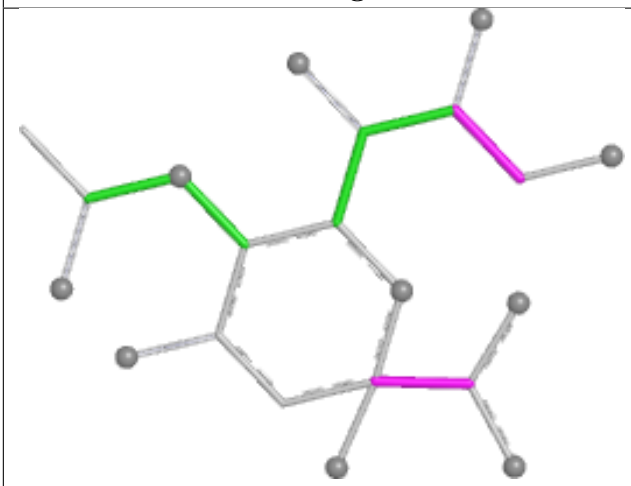
Ligand SIA C 1409



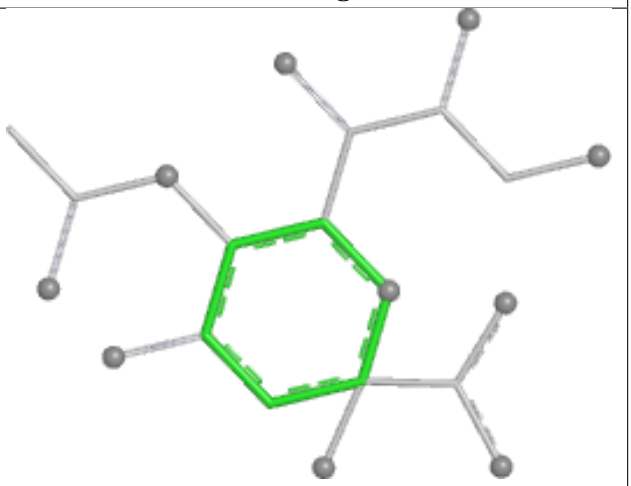
Bond lengths



Bond angles

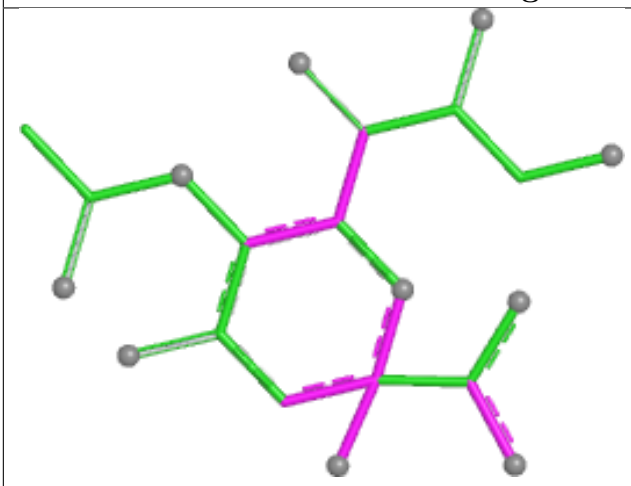


Torsions

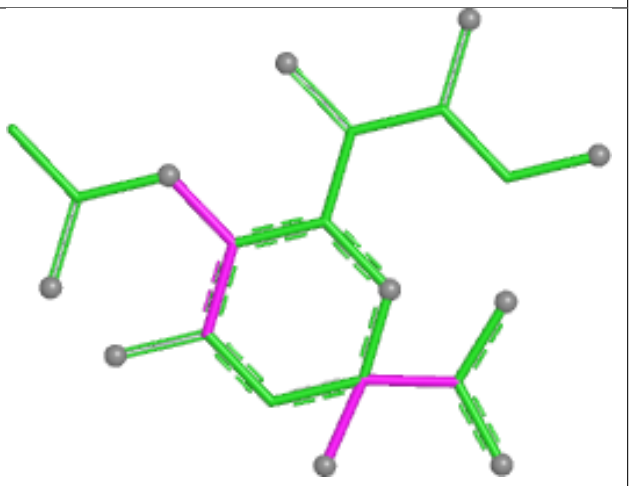


Rings

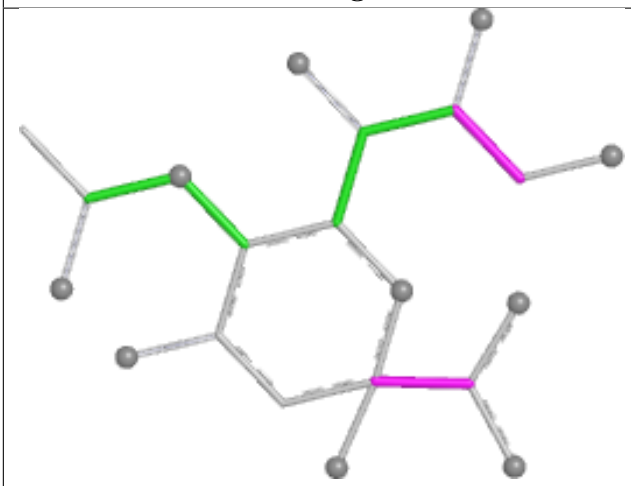
Ligand SIA A 1409



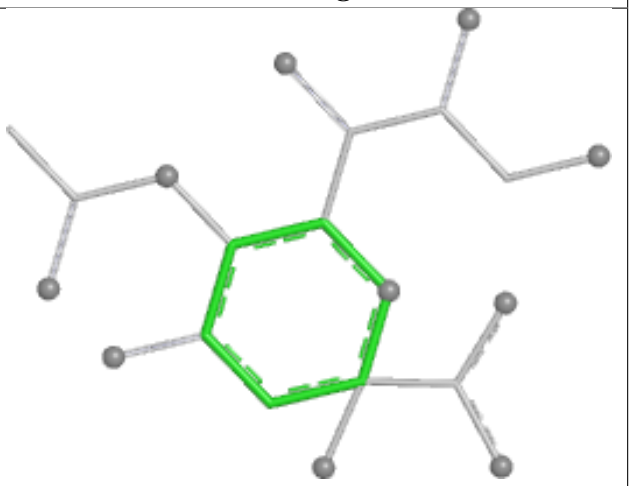
Bond lengths



Bond angles

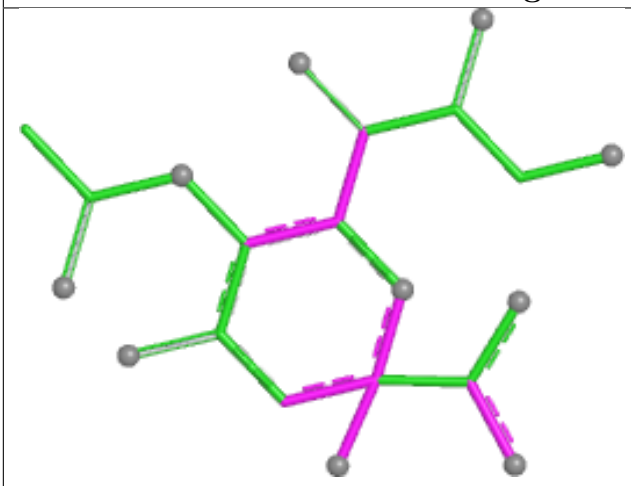


Torsions

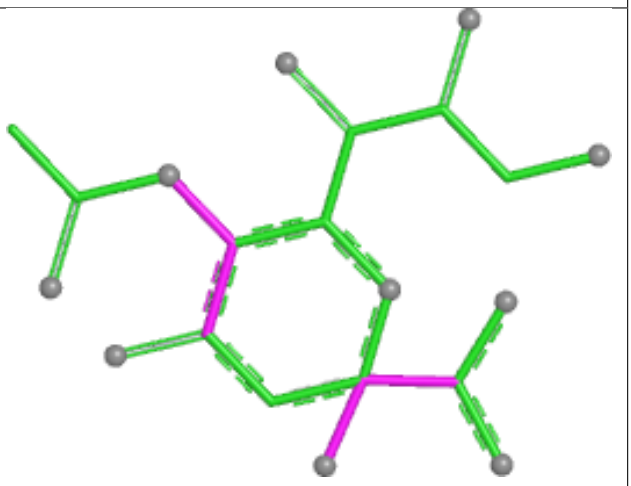


Rings

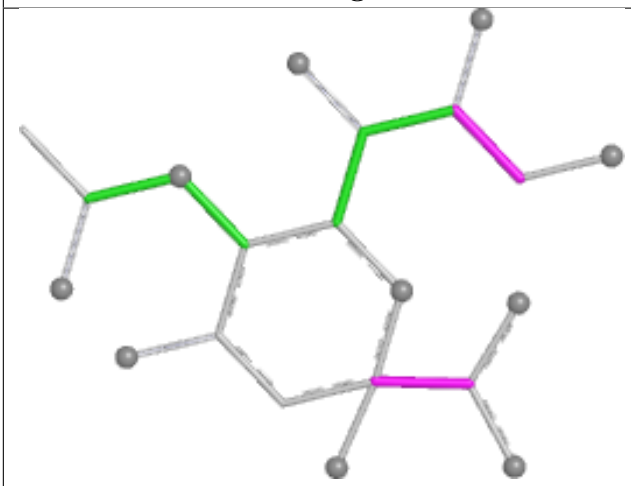
Ligand SIA E 1409



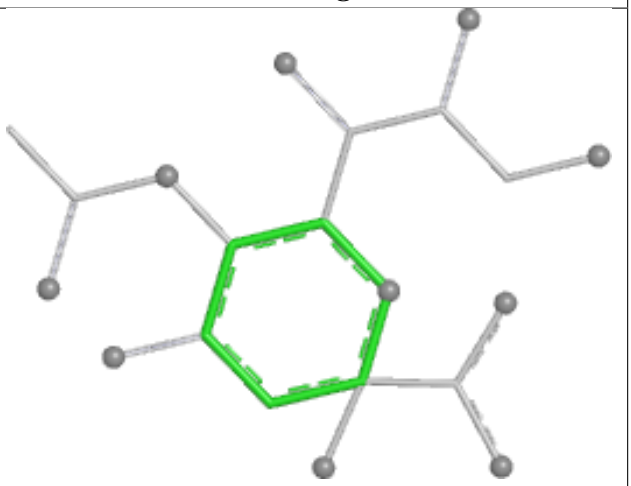
Bond lengths



Bond angles

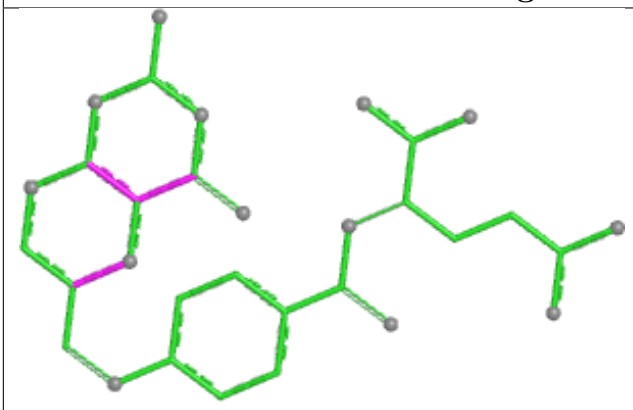


Torsions

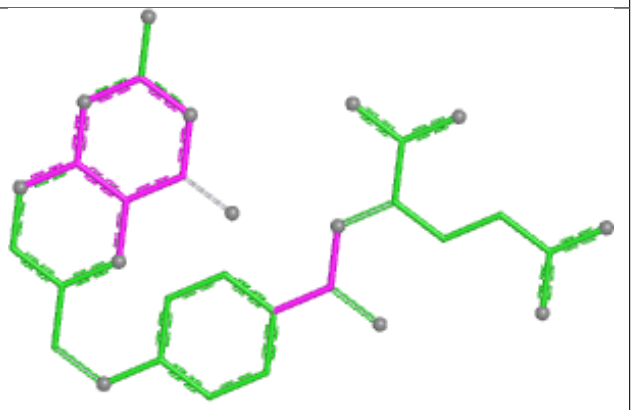


Rings

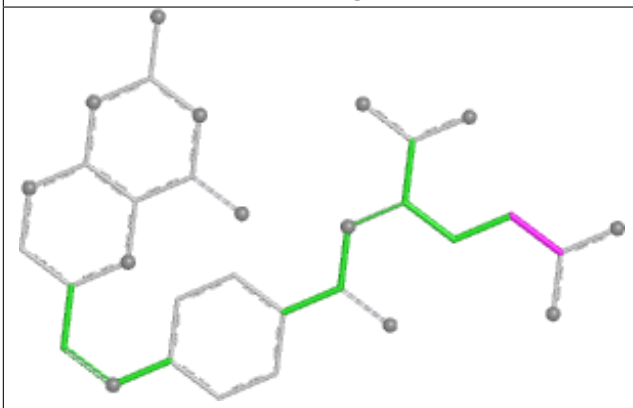
Ligand FOL A 1401



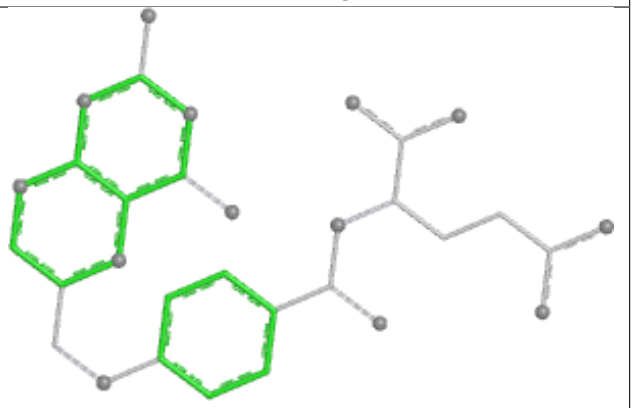
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

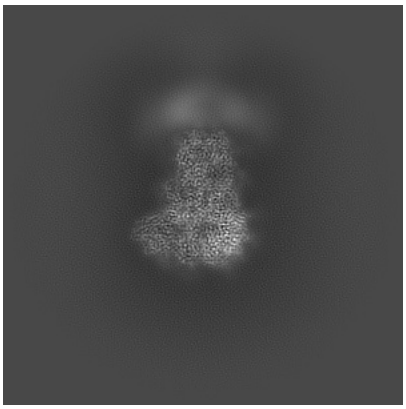
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23674. These allow visual inspection of the internal detail of the map and identification of artifacts.

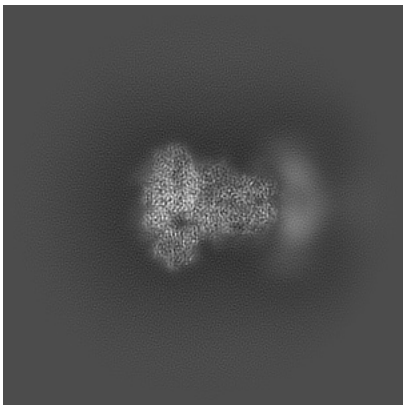
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

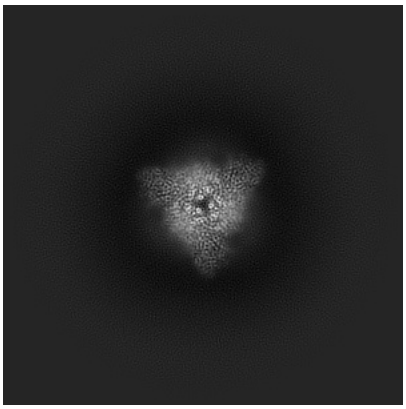
6.1.1 Primary map



X

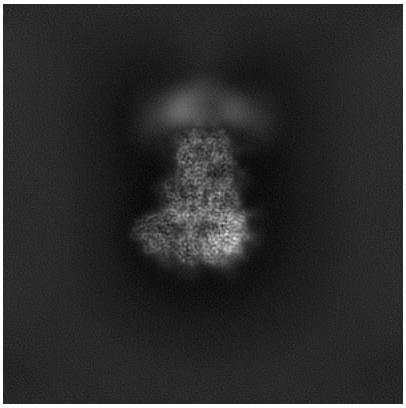


Y

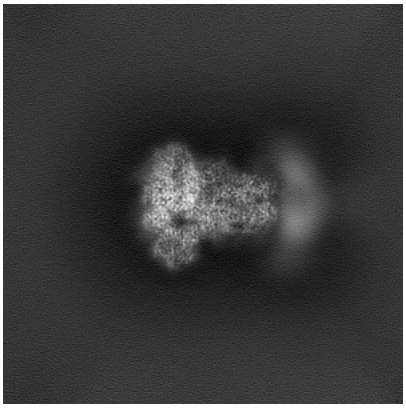


Z

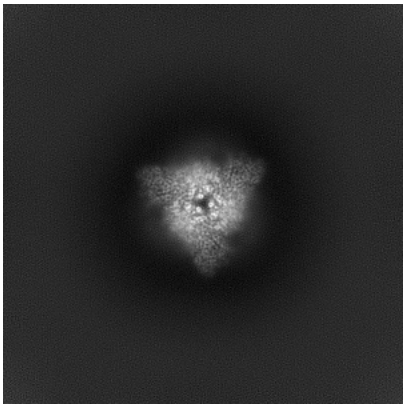
6.1.2 Raw map



X



Y

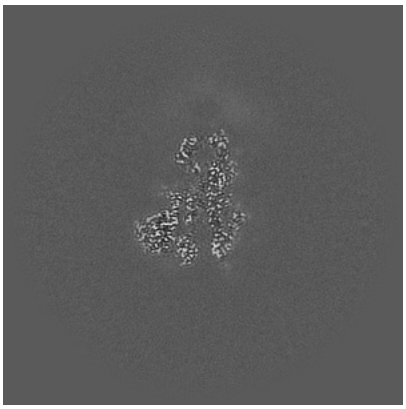


Z

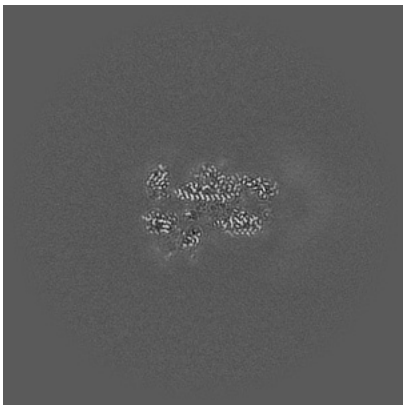
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

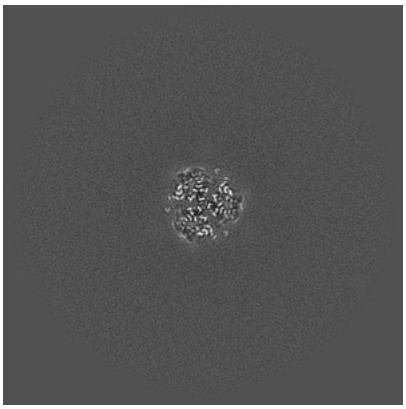
6.2.1 Primary map



X Index: 200

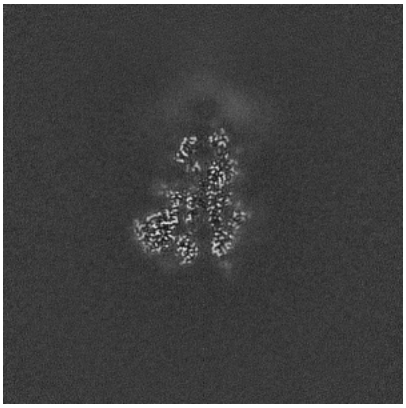


Y Index: 200

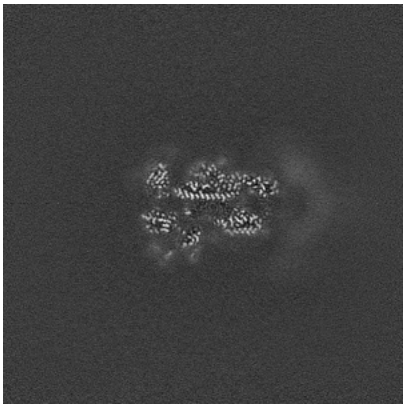


Z Index: 200

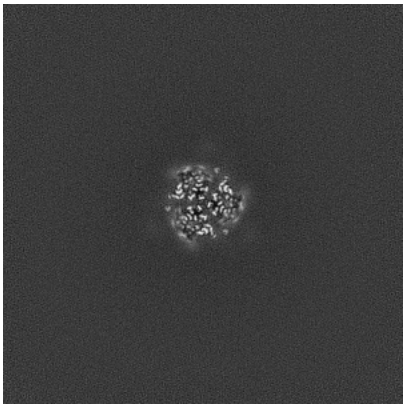
6.2.2 Raw map



X Index: 200



Y Index: 200

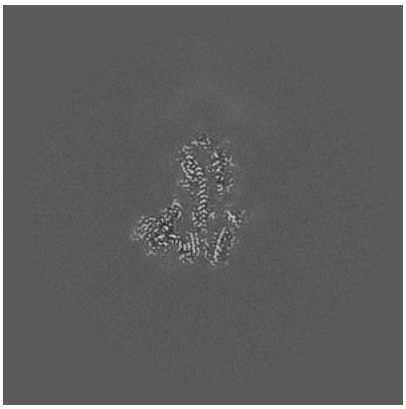


Z Index: 200

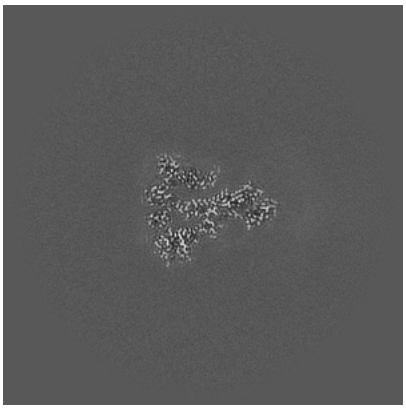
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

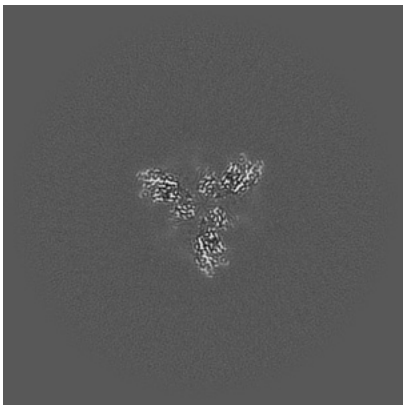
6.3.1 Primary map



X Index: 208

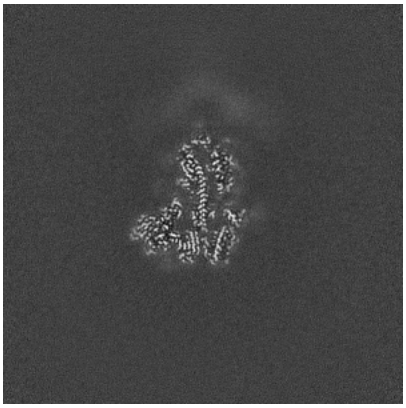


Y Index: 216

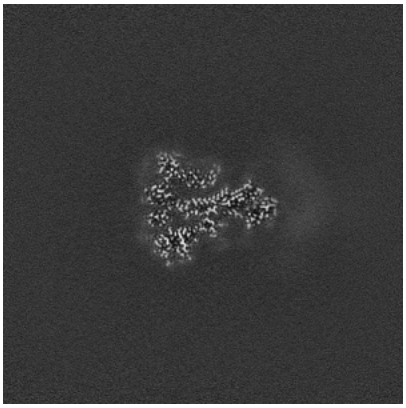


Z Index: 169

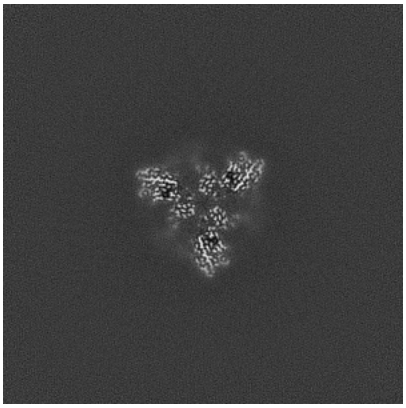
6.3.2 Raw map



X Index: 208



Y Index: 216

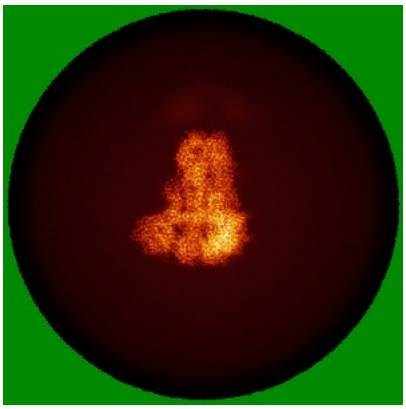


Z Index: 169

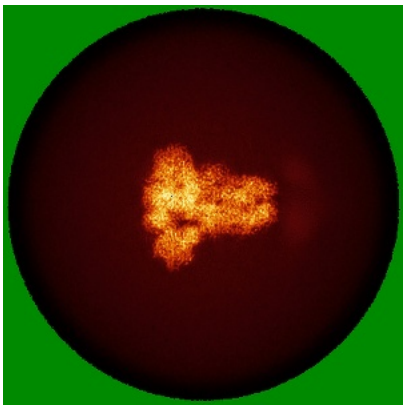
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

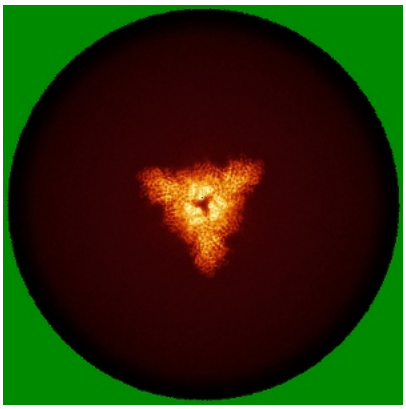
6.4.1 Primary map



X

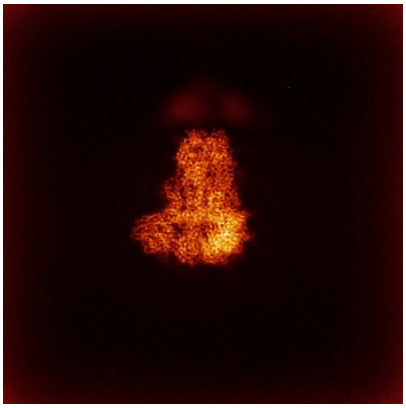


Y

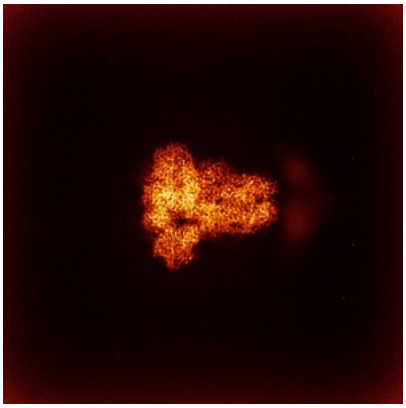


Z

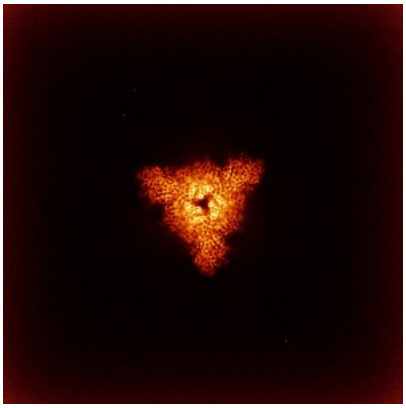
6.4.2 Raw map



X



Y

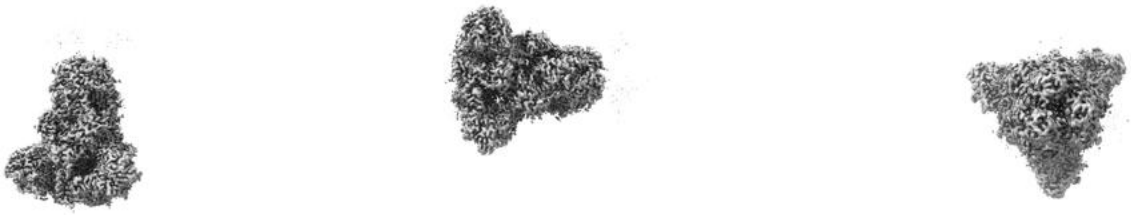


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

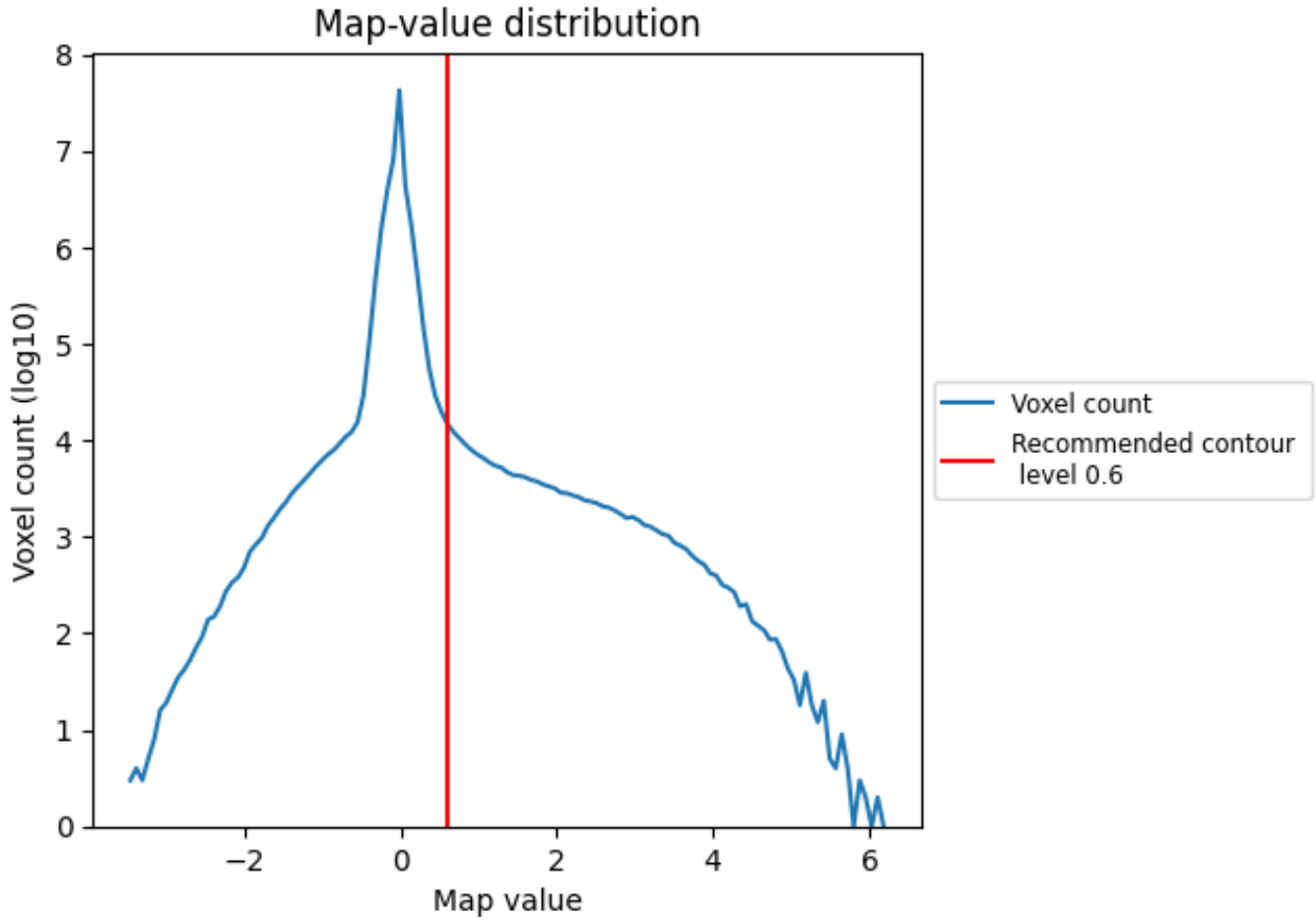
6.6 Mask visualisation (i)

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

7 Map analysis

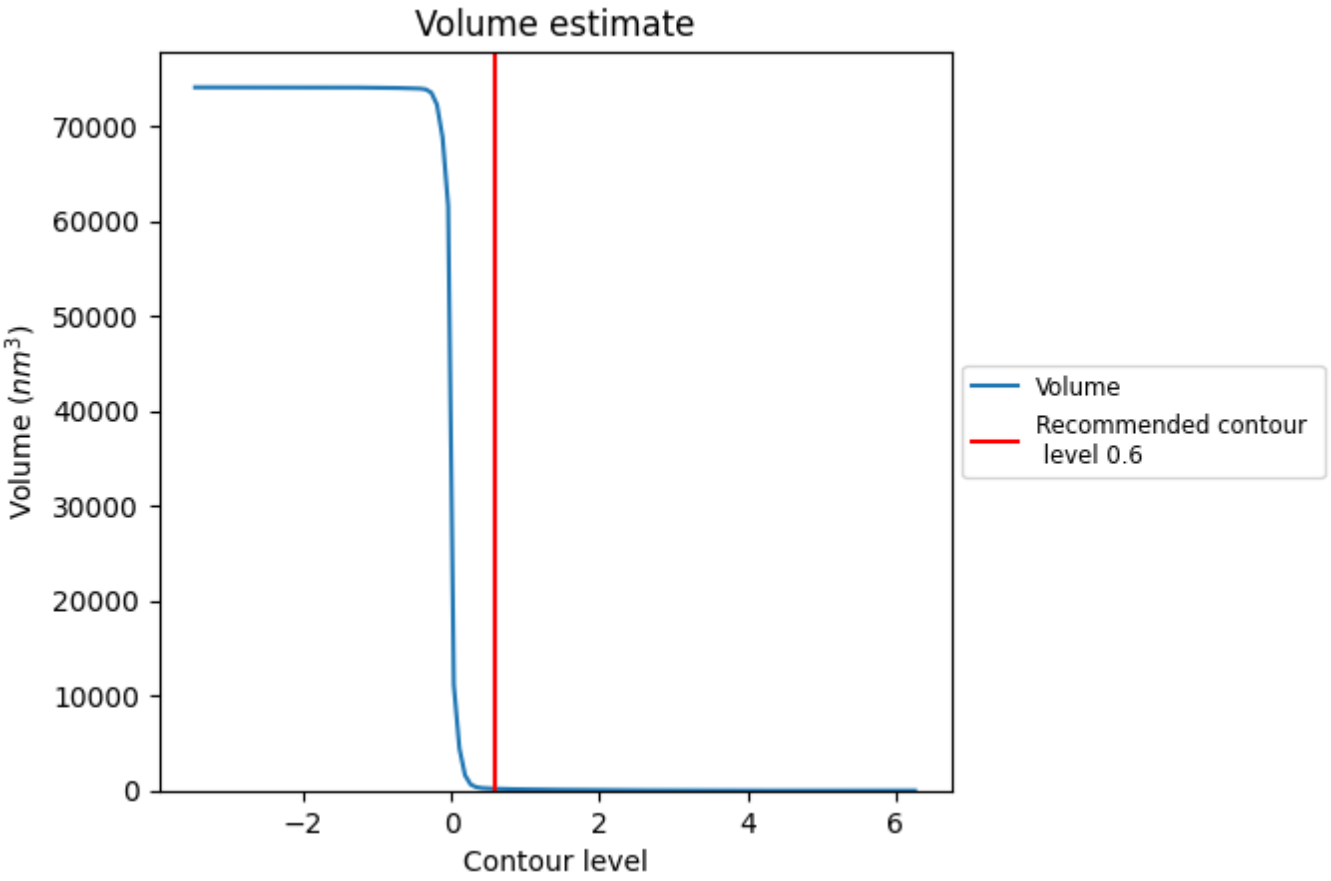
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

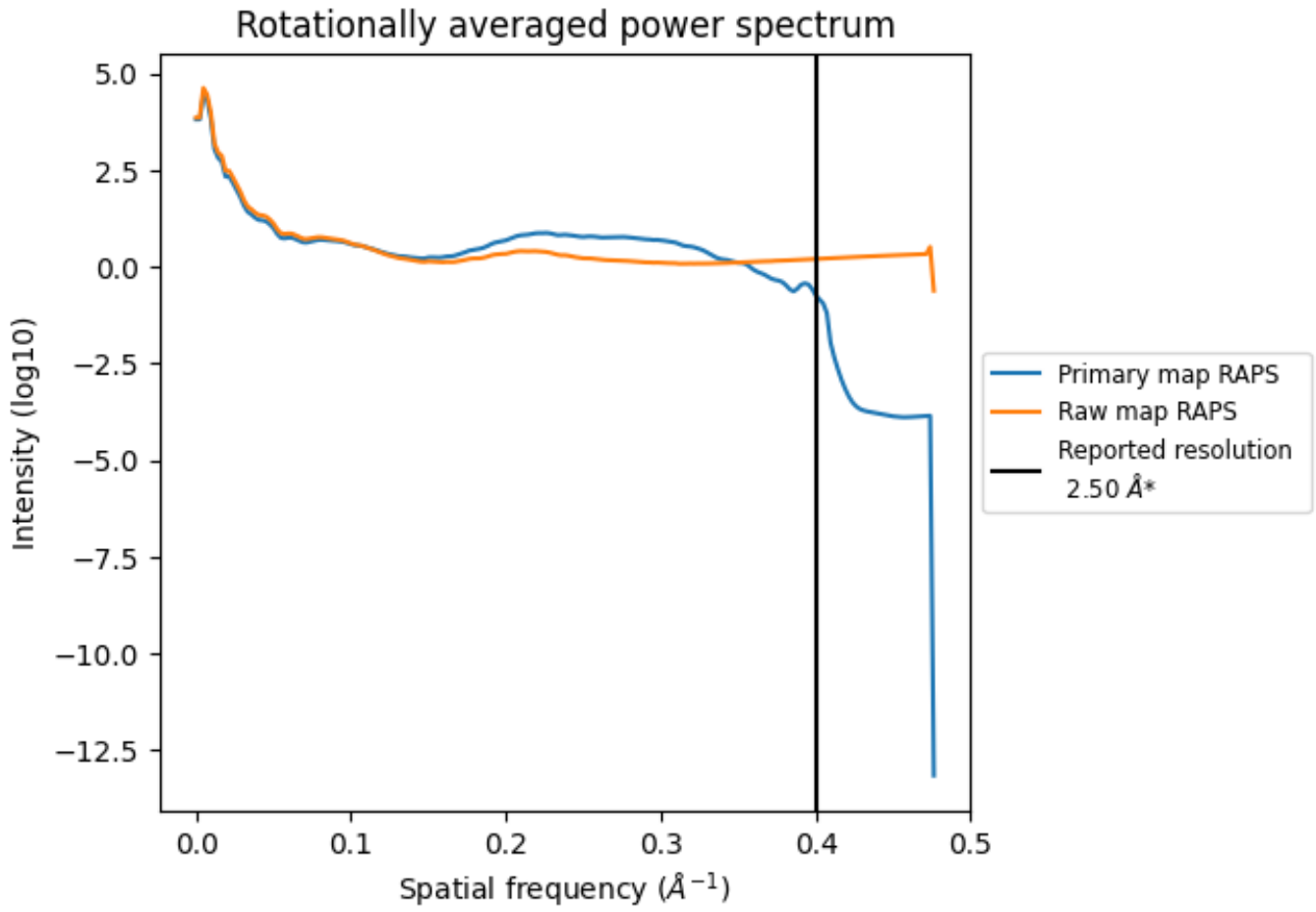
7.2 Volume estimate



The volume at the recommended contour level is 190 nm^3; this corresponds to an approximate mass of 172 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)

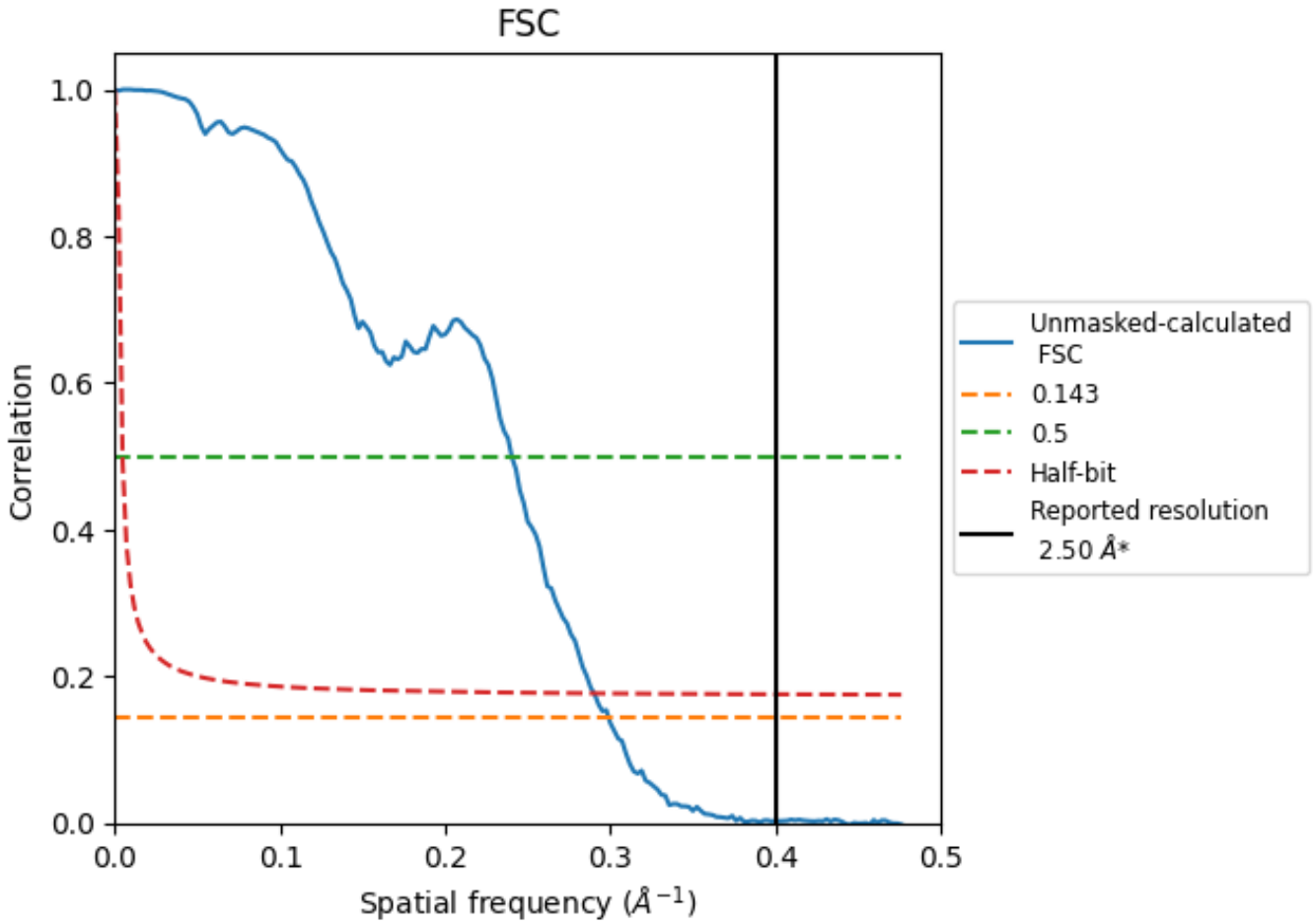


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

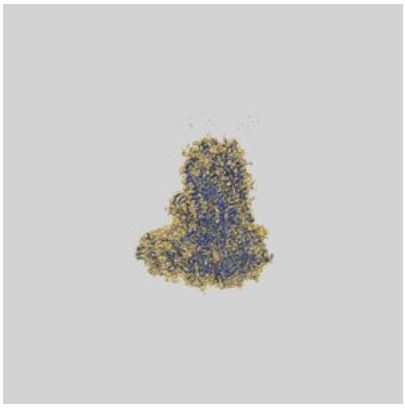
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	4.16	3.45

*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 3.34 differs from the reported value 2.5 by more than 10 %

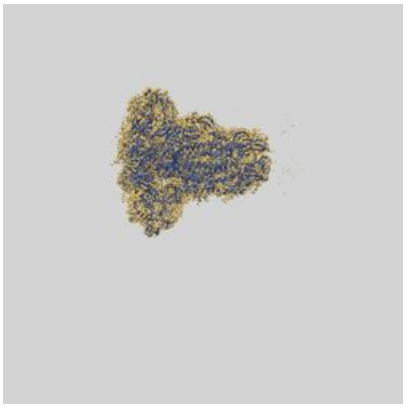
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23674 and PDB model 7M5E. Per-residue inclusion information can be found in section 3 on page 17.

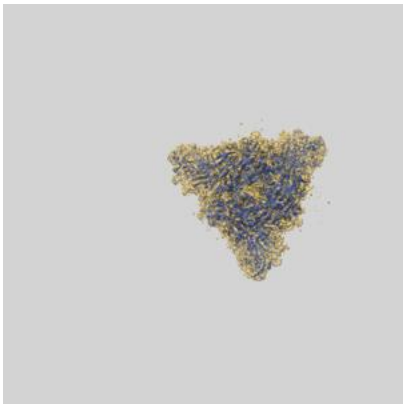
9.1 Map-model overlay



X



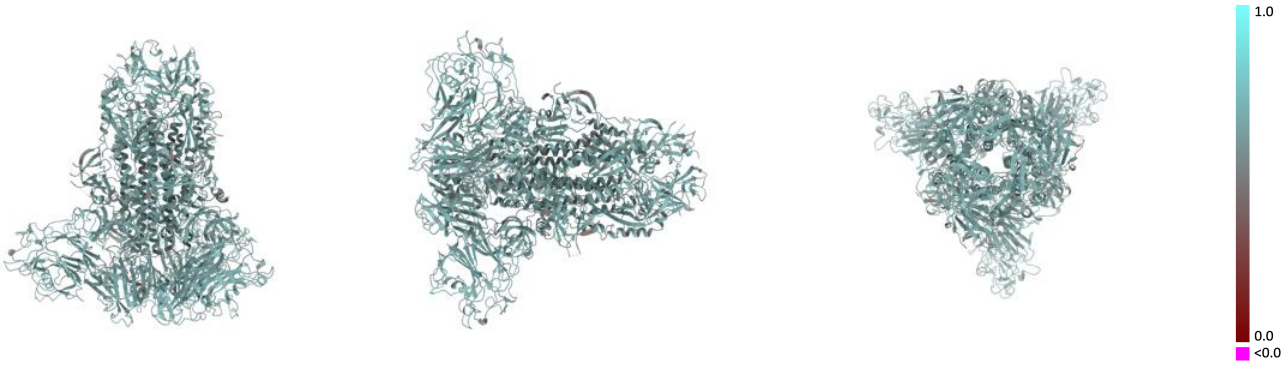
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

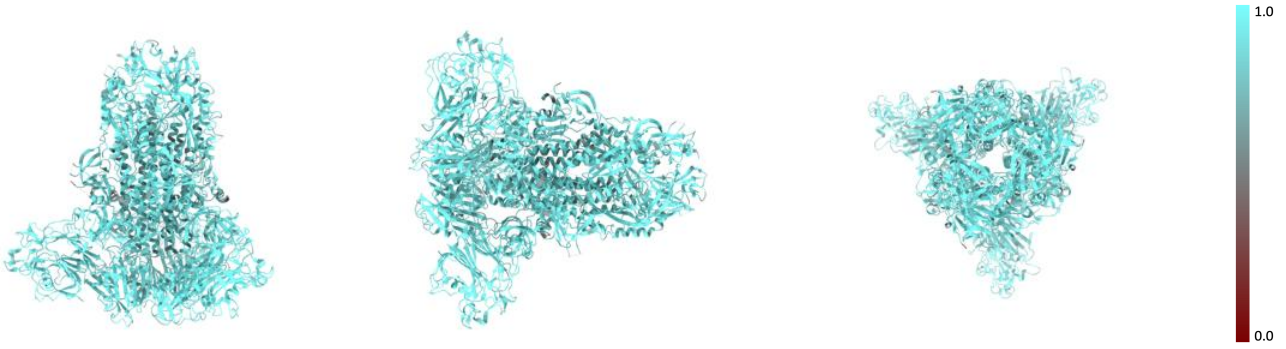
9.2 Q-score mapped to coordinate model (i)



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.

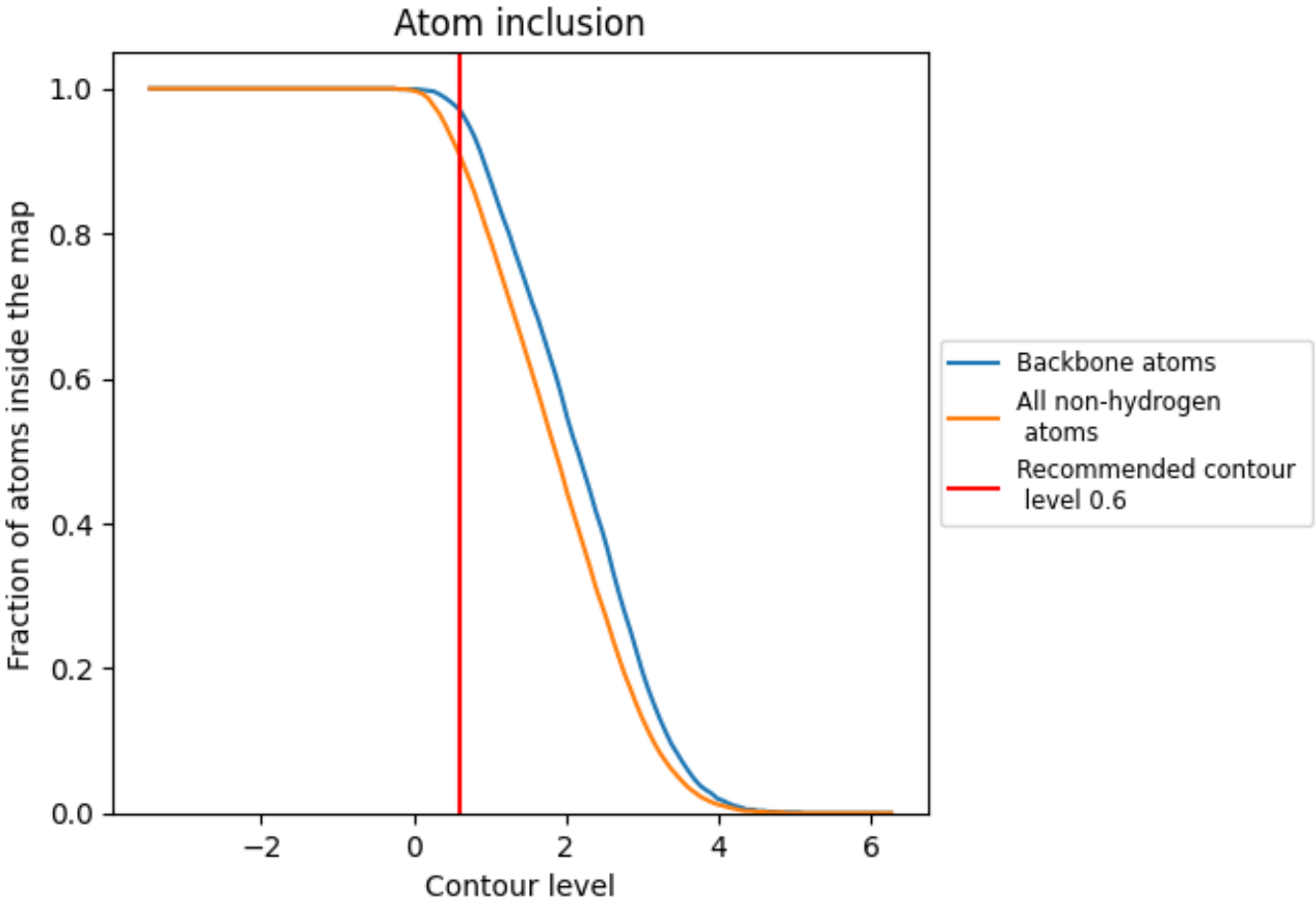
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9090	0.6050
A	0.9270	0.6150
B	0.7400	0.5110
C	0.9260	0.6140
D	0.4640	0.3180
E	0.9260	0.6140
F	0.6510	0.4660
G	0.4100	0.2600
H	0.4800	0.3800
I	0.6790	0.4510
J	0.2500	0.3830
K	0.7050	0.4980
L	0.3930	0.3310
M	0.6070	0.4760
N	0.7400	0.5000
O	0.4640	0.3130
P	0.6390	0.4760
Q	0.4360	0.2520
R	0.4400	0.3760
S	0.6790	0.4490
T	0.2860	0.4010
U	0.7050	0.5030
V	0.3610	0.3410
W	0.6070	0.4520
X	0.7800	0.5040
Y	0.4640	0.3100
Z	0.6750	0.4650
a	0.4360	0.2700
b	0.4600	0.3830
c	0.6790	0.4540
d	0.2500	0.3970
e	0.7050	0.4920
f	0.4260	0.3300
g	0.6070	0.4580