wwPDB EM Validation Summary Report

Sep 28, 2024 – 11:24 PM EDT

PDB ID	:	8EU8
EMDB ID	:	EMD-28608
Title	:	Cryo-EM structure of CH848 10.17DT DS-SOSIP-2P Env
Authors	:	Wrapp, D.; Acharya, P.; Haynes, B.F.
Deposited on	:	2022-10-18
Resolution	:	3.73 Å(reported)

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

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

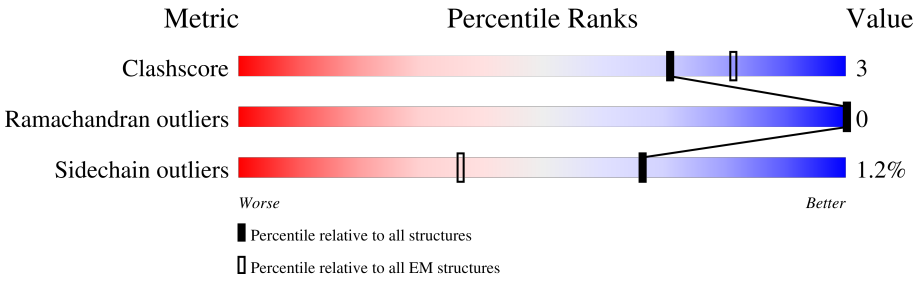
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.73 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.



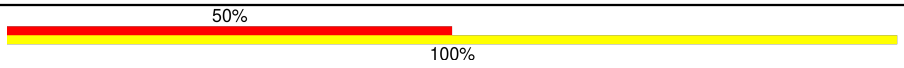
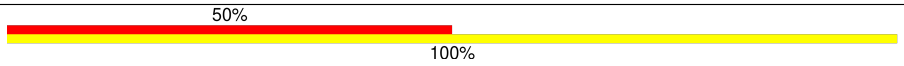
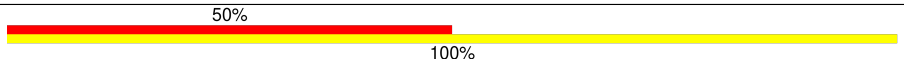
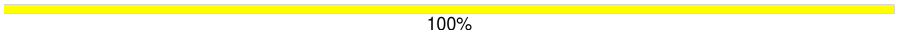
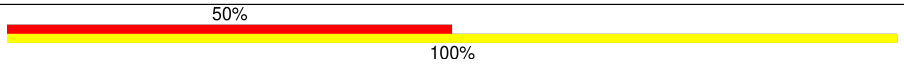
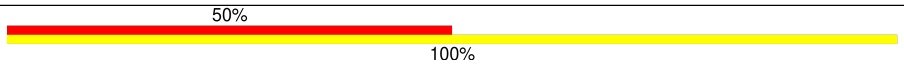
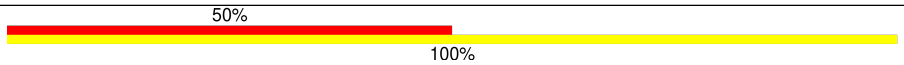
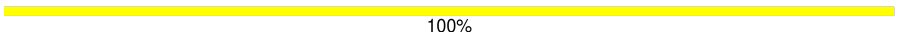
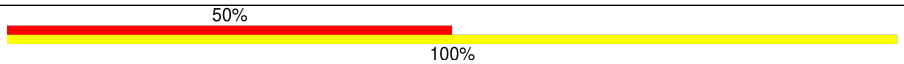
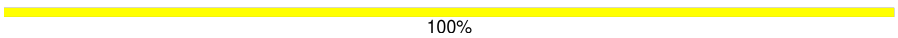
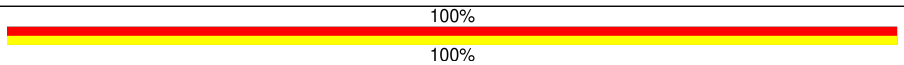
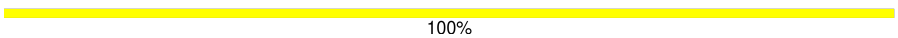
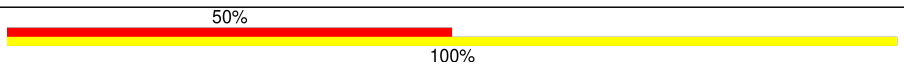
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	698	76% 5% 19%
1	B	698	76% 5% 19%
1	C	698	75% 5% 19%
2	D	2	100%
2	E	2	50% 100%
2	F	2	100%
2	G	2	100% 100%
2	H	2	50% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14181 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 CH848 10.17DT SOSIP Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	564	Total	C	N	O	S	0	0
			4433	2784	765	849	35		
1	B	564	Total	C	N	O	S	0	0
			4433	2784	765	849	35		
1	C	564	Total	C	N	O	S	0	0
			4433	2784	765	849	35		

There are 357 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP A0A1W6IPB2
A	8	PRO	-	expression tag	UNP A0A1W6IPB2
A	9	MET	-	expression tag	UNP A0A1W6IPB2
A	10	GLY	-	expression tag	UNP A0A1W6IPB2
A	11	SER	-	expression tag	UNP A0A1W6IPB2
A	12	LEU	-	expression tag	UNP A0A1W6IPB2
A	13	GLN	-	expression tag	UNP A0A1W6IPB2
A	14	PRO	-	expression tag	UNP A0A1W6IPB2
A	15	LEU	-	expression tag	UNP A0A1W6IPB2
A	16	ALA	-	expression tag	UNP A0A1W6IPB2
A	17	THR	-	expression tag	UNP A0A1W6IPB2
A	18	LEU	-	expression tag	UNP A0A1W6IPB2
A	19	TYR	-	expression tag	UNP A0A1W6IPB2
A	20	LEU	-	expression tag	UNP A0A1W6IPB2
A	21	LEU	-	expression tag	UNP A0A1W6IPB2
A	22	GLY	-	expression tag	UNP A0A1W6IPB2
A	23	MET	-	expression tag	UNP A0A1W6IPB2
A	24	LEU	-	expression tag	UNP A0A1W6IPB2
A	25	VAL	-	expression tag	UNP A0A1W6IPB2
A	26	ALA	-	expression tag	UNP A0A1W6IPB2
A	27	SER	-	expression tag	UNP A0A1W6IPB2
A	28	VAL	-	expression tag	UNP A0A1W6IPB2
A	29	LEU	-	expression tag	UNP A0A1W6IPB2
A	30	ALA	-	expression tag	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP A0A1W6IPB2
A	32	GLU	-	expression tag	UNP A0A1W6IPB2
A	33	ASN	-	expression tag	UNP A0A1W6IPB2
A	133	ASP	ASN	conflict	UNP A0A1W6IPB2
A	138	THR	ASN	conflict	UNP A0A1W6IPB2
A	201	CYS	VAL	conflict	UNP A0A1W6IPB2
A	433	CYS	ALA	conflict	UNP A0A1W6IPB2
A	490	LYS	GLU	conflict	UNP A0A1W6IPB2
A	492	GLU	GLN	conflict	UNP A0A1W6IPB2
A	496	VAL	ILE	conflict	UNP A0A1W6IPB2
A	500	ARG	GLY	conflict	UNP A0A1W6IPB2
A	501	CYS	ALA	conflict	UNP A0A1W6IPB2
A	505B	GLY	-	insertion	UNP A0A1W6IPB2
A	505C	ARG	-	insertion	UNP A0A1W6IPB2
A	505D	ARG	GLU	conflict	UNP A0A1W6IPB2
A	505F	ARG	GLU	conflict	UNP A0A1W6IPB2
A	505G	ARG	LYS	conflict	UNP A0A1W6IPB2
A	505J	VAL	ALA	conflict	UNP A0A1W6IPB2
A	505L	ILE	LEU	conflict	UNP A0A1W6IPB2
A	505O	VAL	LEU	conflict	UNP A0A1W6IPB2
A	535	MET	ILE	conflict	UNP A0A1W6IPB2
A	543	ASN	GLN	conflict	UNP A0A1W6IPB2
A	559	PRO	ILE	engineered mutation	UNP A0A1W6IPB2
A	565	LEU	MET	conflict	UNP A0A1W6IPB2
A	567	LYS	GLN	conflict	UNP A0A1W6IPB2
A	568	PRO	LEU	conflict	UNP A0A1W6IPB2
A	569	PRO	THR	conflict	UNP A0A1W6IPB2
A	583	VAL	LEU	conflict	UNP A0A1W6IPB2
A	588	ARG	LYS	conflict	UNP A0A1W6IPB2
A	595	ILE	MET	conflict	UNP A0A1W6IPB2
A	605	CYS	THR	conflict	UNP A0A1W6IPB2
A	612	SER	THR	conflict	UNP A0A1W6IPB2
A	617	ARG	LYS	conflict	UNP A0A1W6IPB2
A	618	ASN	SER	conflict	UNP A0A1W6IPB2
A	619	LEU	GLU	conflict	UNP A0A1W6IPB2
A	620	SER	THR	conflict	UNP A0A1W6IPB2
A	621	GLU	ASP	conflict	UNP A0A1W6IPB2
A	629	LEU	MET	conflict	UNP A0A1W6IPB2
A	632	ASP	GLU	conflict	UNP A0A1W6IPB2
A	633	LYS	ARG	conflict	UNP A0A1W6IPB2
A	640	GLN	GLU	conflict	UNP A0A1W6IPB2
A	641	ILE	THR	conflict	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	644	GLY	LYS	conflict	UNP A0A1W6IPB2
A	648	GLU	ASP	conflict	UNP A0A1W6IPB2
A	655	LYS	ARG	conflict	UNP A0A1W6IPB2
A	665	GLY	-	expression tag	UNP A0A1W6IPB2
A	666	SER	-	expression tag	UNP A0A1W6IPB2
A	667	LEU	-	expression tag	UNP A0A1W6IPB2
A	668	GLU	-	expression tag	UNP A0A1W6IPB2
A	669	VAL	-	expression tag	UNP A0A1W6IPB2
A	670	LEU	-	expression tag	UNP A0A1W6IPB2
A	671	PHE	-	expression tag	UNP A0A1W6IPB2
A	672	GLN	-	expression tag	UNP A0A1W6IPB2
A	673	GLY	-	expression tag	UNP A0A1W6IPB2
A	674	PRO	-	expression tag	UNP A0A1W6IPB2
A	675	GLY	-	expression tag	UNP A0A1W6IPB2
A	676	HIS	-	expression tag	UNP A0A1W6IPB2
A	677	HIS	-	expression tag	UNP A0A1W6IPB2
A	678	HIS	-	expression tag	UNP A0A1W6IPB2
A	679	HIS	-	expression tag	UNP A0A1W6IPB2
A	680	HIS	-	expression tag	UNP A0A1W6IPB2
A	681	HIS	-	expression tag	UNP A0A1W6IPB2
A	682	HIS	-	expression tag	UNP A0A1W6IPB2
A	683	HIS	-	expression tag	UNP A0A1W6IPB2
A	684	SER	-	expression tag	UNP A0A1W6IPB2
A	685	ALA	-	expression tag	UNP A0A1W6IPB2
A	686	TRP	-	expression tag	UNP A0A1W6IPB2
A	687	SER	-	expression tag	UNP A0A1W6IPB2
A	688	HIS	-	expression tag	UNP A0A1W6IPB2
A	689	PRO	-	expression tag	UNP A0A1W6IPB2
A	690	GLN	-	expression tag	UNP A0A1W6IPB2
A	691	PHE	-	expression tag	UNP A0A1W6IPB2
A	692	GLU	-	expression tag	UNP A0A1W6IPB2
A	693	LYS	-	expression tag	UNP A0A1W6IPB2
A	694	GLY	-	expression tag	UNP A0A1W6IPB2
A	695	GLY	-	expression tag	UNP A0A1W6IPB2
A	696	GLY	-	expression tag	UNP A0A1W6IPB2
A	697	SER	-	expression tag	UNP A0A1W6IPB2
A	698	GLY	-	expression tag	UNP A0A1W6IPB2
A	699	GLY	-	expression tag	UNP A0A1W6IPB2
A	700	GLY	-	expression tag	UNP A0A1W6IPB2
A	701	GLY	-	expression tag	UNP A0A1W6IPB2
A	702	SER	-	expression tag	UNP A0A1W6IPB2
A	703	GLY	-	expression tag	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	GLY	-	expression tag	UNP A0A1W6IPB2
A	705	SER	-	expression tag	UNP A0A1W6IPB2
A	706	ALA	-	expression tag	UNP A0A1W6IPB2
A	707	TRP	-	expression tag	UNP A0A1W6IPB2
A	708	SER	-	expression tag	UNP A0A1W6IPB2
A	709	HIS	-	expression tag	UNP A0A1W6IPB2
A	710	PRO	-	expression tag	UNP A0A1W6IPB2
A	711	GLN	-	expression tag	UNP A0A1W6IPB2
A	712	PHE	-	expression tag	UNP A0A1W6IPB2
A	713	GLU	-	expression tag	UNP A0A1W6IPB2
A	714	LYS	-	expression tag	UNP A0A1W6IPB2
B	7	MET	-	initiating methionine	UNP A0A1W6IPB2
B	8	PRO	-	expression tag	UNP A0A1W6IPB2
B	9	MET	-	expression tag	UNP A0A1W6IPB2
B	10	GLY	-	expression tag	UNP A0A1W6IPB2
B	11	SER	-	expression tag	UNP A0A1W6IPB2
B	12	LEU	-	expression tag	UNP A0A1W6IPB2
B	13	GLN	-	expression tag	UNP A0A1W6IPB2
B	14	PRO	-	expression tag	UNP A0A1W6IPB2
B	15	LEU	-	expression tag	UNP A0A1W6IPB2
B	16	ALA	-	expression tag	UNP A0A1W6IPB2
B	17	THR	-	expression tag	UNP A0A1W6IPB2
B	18	LEU	-	expression tag	UNP A0A1W6IPB2
B	19	TYR	-	expression tag	UNP A0A1W6IPB2
B	20	LEU	-	expression tag	UNP A0A1W6IPB2
B	21	LEU	-	expression tag	UNP A0A1W6IPB2
B	22	GLY	-	expression tag	UNP A0A1W6IPB2
B	23	MET	-	expression tag	UNP A0A1W6IPB2
B	24	LEU	-	expression tag	UNP A0A1W6IPB2
B	25	VAL	-	expression tag	UNP A0A1W6IPB2
B	26	ALA	-	expression tag	UNP A0A1W6IPB2
B	27	SER	-	expression tag	UNP A0A1W6IPB2
B	28	VAL	-	expression tag	UNP A0A1W6IPB2
B	29	LEU	-	expression tag	UNP A0A1W6IPB2
B	30	ALA	-	expression tag	UNP A0A1W6IPB2
B	31	ALA	-	expression tag	UNP A0A1W6IPB2
B	32	GLU	-	expression tag	UNP A0A1W6IPB2
B	33	ASN	-	expression tag	UNP A0A1W6IPB2
B	133	ASP	ASN	conflict	UNP A0A1W6IPB2
B	138	THR	ASN	conflict	UNP A0A1W6IPB2
B	201	CYS	VAL	conflict	UNP A0A1W6IPB2
B	433	CYS	ALA	conflict	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	490	LYS	GLU	conflict	UNP A0A1W6IPB2
B	492	GLU	GLN	conflict	UNP A0A1W6IPB2
B	496	VAL	ILE	conflict	UNP A0A1W6IPB2
B	500	ARG	GLY	conflict	UNP A0A1W6IPB2
B	501	CYS	ALA	conflict	UNP A0A1W6IPB2
B	505B	GLY	-	insertion	UNP A0A1W6IPB2
B	505C	ARG	-	insertion	UNP A0A1W6IPB2
B	505D	ARG	GLU	conflict	UNP A0A1W6IPB2
B	505F	ARG	GLU	conflict	UNP A0A1W6IPB2
B	505G	ARG	LYS	conflict	UNP A0A1W6IPB2
B	505J	VAL	ALA	conflict	UNP A0A1W6IPB2
B	505L	ILE	LEU	conflict	UNP A0A1W6IPB2
B	505O	VAL	LEU	conflict	UNP A0A1W6IPB2
B	535	MET	ILE	conflict	UNP A0A1W6IPB2
B	543	ASN	GLN	conflict	UNP A0A1W6IPB2
B	559	PRO	ILE	engineered mutation	UNP A0A1W6IPB2
B	565	LEU	MET	conflict	UNP A0A1W6IPB2
B	567	LYS	GLN	conflict	UNP A0A1W6IPB2
B	568	PRO	LEU	conflict	UNP A0A1W6IPB2
B	569	PRO	THR	conflict	UNP A0A1W6IPB2
B	583	VAL	LEU	conflict	UNP A0A1W6IPB2
B	588	ARG	LYS	conflict	UNP A0A1W6IPB2
B	595	ILE	MET	conflict	UNP A0A1W6IPB2
B	605	CYS	THR	conflict	UNP A0A1W6IPB2
B	612	SER	THR	conflict	UNP A0A1W6IPB2
B	617	ARG	LYS	conflict	UNP A0A1W6IPB2
B	618	ASN	SER	conflict	UNP A0A1W6IPB2
B	619	LEU	GLU	conflict	UNP A0A1W6IPB2
B	620	SER	THR	conflict	UNP A0A1W6IPB2
B	621	GLU	ASP	conflict	UNP A0A1W6IPB2
B	629	LEU	MET	conflict	UNP A0A1W6IPB2
B	632	ASP	GLU	conflict	UNP A0A1W6IPB2
B	633	LYS	ARG	conflict	UNP A0A1W6IPB2
B	640	GLN	GLU	conflict	UNP A0A1W6IPB2
B	641	ILE	THR	conflict	UNP A0A1W6IPB2
B	644	GLY	LYS	conflict	UNP A0A1W6IPB2
B	648	GLU	ASP	conflict	UNP A0A1W6IPB2
B	655	LYS	ARG	conflict	UNP A0A1W6IPB2
B	665	GLY	-	expression tag	UNP A0A1W6IPB2
B	666	SER	-	expression tag	UNP A0A1W6IPB2
B	667	LEU	-	expression tag	UNP A0A1W6IPB2
B	668	GLU	-	expression tag	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	669	VAL	-	expression tag	UNP A0A1W6IPB2
B	670	LEU	-	expression tag	UNP A0A1W6IPB2
B	671	PHE	-	expression tag	UNP A0A1W6IPB2
B	672	GLN	-	expression tag	UNP A0A1W6IPB2
B	673	GLY	-	expression tag	UNP A0A1W6IPB2
B	674	PRO	-	expression tag	UNP A0A1W6IPB2
B	675	GLY	-	expression tag	UNP A0A1W6IPB2
B	676	HIS	-	expression tag	UNP A0A1W6IPB2
B	677	HIS	-	expression tag	UNP A0A1W6IPB2
B	678	HIS	-	expression tag	UNP A0A1W6IPB2
B	679	HIS	-	expression tag	UNP A0A1W6IPB2
B	680	HIS	-	expression tag	UNP A0A1W6IPB2
B	681	HIS	-	expression tag	UNP A0A1W6IPB2
B	682	HIS	-	expression tag	UNP A0A1W6IPB2
B	683	HIS	-	expression tag	UNP A0A1W6IPB2
B	684	SER	-	expression tag	UNP A0A1W6IPB2
B	685	ALA	-	expression tag	UNP A0A1W6IPB2
B	686	TRP	-	expression tag	UNP A0A1W6IPB2
B	687	SER	-	expression tag	UNP A0A1W6IPB2
B	688	HIS	-	expression tag	UNP A0A1W6IPB2
B	689	PRO	-	expression tag	UNP A0A1W6IPB2
B	690	GLN	-	expression tag	UNP A0A1W6IPB2
B	691	PHE	-	expression tag	UNP A0A1W6IPB2
B	692	GLU	-	expression tag	UNP A0A1W6IPB2
B	693	LYS	-	expression tag	UNP A0A1W6IPB2
B	694	GLY	-	expression tag	UNP A0A1W6IPB2
B	695	GLY	-	expression tag	UNP A0A1W6IPB2
B	696	GLY	-	expression tag	UNP A0A1W6IPB2
B	697	SER	-	expression tag	UNP A0A1W6IPB2
B	698	GLY	-	expression tag	UNP A0A1W6IPB2
B	699	GLY	-	expression tag	UNP A0A1W6IPB2
B	700	GLY	-	expression tag	UNP A0A1W6IPB2
B	701	GLY	-	expression tag	UNP A0A1W6IPB2
B	702	SER	-	expression tag	UNP A0A1W6IPB2
B	703	GLY	-	expression tag	UNP A0A1W6IPB2
B	704	GLY	-	expression tag	UNP A0A1W6IPB2
B	705	SER	-	expression tag	UNP A0A1W6IPB2
B	706	ALA	-	expression tag	UNP A0A1W6IPB2
B	707	TRP	-	expression tag	UNP A0A1W6IPB2
B	708	SER	-	expression tag	UNP A0A1W6IPB2
B	709	HIS	-	expression tag	UNP A0A1W6IPB2
B	710	PRO	-	expression tag	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	711	GLN	-	expression tag	UNP A0A1W6IPB2
B	712	PHE	-	expression tag	UNP A0A1W6IPB2
B	713	GLU	-	expression tag	UNP A0A1W6IPB2
B	714	LYS	-	expression tag	UNP A0A1W6IPB2
C	7	MET	-	initiating methionine	UNP A0A1W6IPB2
C	8	PRO	-	expression tag	UNP A0A1W6IPB2
C	9	MET	-	expression tag	UNP A0A1W6IPB2
C	10	GLY	-	expression tag	UNP A0A1W6IPB2
C	11	SER	-	expression tag	UNP A0A1W6IPB2
C	12	LEU	-	expression tag	UNP A0A1W6IPB2
C	13	GLN	-	expression tag	UNP A0A1W6IPB2
C	14	PRO	-	expression tag	UNP A0A1W6IPB2
C	15	LEU	-	expression tag	UNP A0A1W6IPB2
C	16	ALA	-	expression tag	UNP A0A1W6IPB2
C	17	THR	-	expression tag	UNP A0A1W6IPB2
C	18	LEU	-	expression tag	UNP A0A1W6IPB2
C	19	TYR	-	expression tag	UNP A0A1W6IPB2
C	20	LEU	-	expression tag	UNP A0A1W6IPB2
C	21	LEU	-	expression tag	UNP A0A1W6IPB2
C	22	GLY	-	expression tag	UNP A0A1W6IPB2
C	23	MET	-	expression tag	UNP A0A1W6IPB2
C	24	LEU	-	expression tag	UNP A0A1W6IPB2
C	25	VAL	-	expression tag	UNP A0A1W6IPB2
C	26	ALA	-	expression tag	UNP A0A1W6IPB2
C	27	SER	-	expression tag	UNP A0A1W6IPB2
C	28	VAL	-	expression tag	UNP A0A1W6IPB2
C	29	LEU	-	expression tag	UNP A0A1W6IPB2
C	30	ALA	-	expression tag	UNP A0A1W6IPB2
C	31	ALA	-	expression tag	UNP A0A1W6IPB2
C	32	GLU	-	expression tag	UNP A0A1W6IPB2
C	33	ASN	-	expression tag	UNP A0A1W6IPB2
C	133	ASP	ASN	conflict	UNP A0A1W6IPB2
C	138	THR	ASN	conflict	UNP A0A1W6IPB2
C	201	CYS	VAL	conflict	UNP A0A1W6IPB2
C	433	CYS	ALA	conflict	UNP A0A1W6IPB2
C	490	LYS	GLU	conflict	UNP A0A1W6IPB2
C	492	GLU	GLN	conflict	UNP A0A1W6IPB2
C	496	VAL	ILE	conflict	UNP A0A1W6IPB2
C	500	ARG	GLY	conflict	UNP A0A1W6IPB2
C	501	CYS	ALA	conflict	UNP A0A1W6IPB2
C	505B	GLY	-	insertion	UNP A0A1W6IPB2
C	505C	ARG	-	insertion	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	505D	ARG	GLU	conflict	UNP A0A1W6IPB2
C	505F	ARG	GLU	conflict	UNP A0A1W6IPB2
C	505G	ARG	LYS	conflict	UNP A0A1W6IPB2
C	505J	VAL	ALA	conflict	UNP A0A1W6IPB2
C	505L	ILE	LEU	conflict	UNP A0A1W6IPB2
C	505O	VAL	LEU	conflict	UNP A0A1W6IPB2
C	535	MET	ILE	conflict	UNP A0A1W6IPB2
C	543	ASN	GLN	conflict	UNP A0A1W6IPB2
C	559	PRO	ILE	engineered mutation	UNP A0A1W6IPB2
C	565	LEU	MET	conflict	UNP A0A1W6IPB2
C	567	LYS	GLN	conflict	UNP A0A1W6IPB2
C	568	PRO	LEU	conflict	UNP A0A1W6IPB2
C	569	PRO	THR	conflict	UNP A0A1W6IPB2
C	583	VAL	LEU	conflict	UNP A0A1W6IPB2
C	588	ARG	LYS	conflict	UNP A0A1W6IPB2
C	595	ILE	MET	conflict	UNP A0A1W6IPB2
C	605	CYS	THR	conflict	UNP A0A1W6IPB2
C	612	SER	THR	conflict	UNP A0A1W6IPB2
C	617	ARG	LYS	conflict	UNP A0A1W6IPB2
C	618	ASN	SER	conflict	UNP A0A1W6IPB2
C	619	LEU	GLU	conflict	UNP A0A1W6IPB2
C	620	SER	THR	conflict	UNP A0A1W6IPB2
C	621	GLU	ASP	conflict	UNP A0A1W6IPB2
C	629	LEU	MET	conflict	UNP A0A1W6IPB2
C	632	ASP	GLU	conflict	UNP A0A1W6IPB2
C	633	LYS	ARG	conflict	UNP A0A1W6IPB2
C	640	GLN	GLU	conflict	UNP A0A1W6IPB2
C	641	ILE	THR	conflict	UNP A0A1W6IPB2
C	644	GLY	LYS	conflict	UNP A0A1W6IPB2
C	648	GLU	ASP	conflict	UNP A0A1W6IPB2
C	655	LYS	ARG	conflict	UNP A0A1W6IPB2
C	665	GLY	-	expression tag	UNP A0A1W6IPB2
C	666	SER	-	expression tag	UNP A0A1W6IPB2
C	667	LEU	-	expression tag	UNP A0A1W6IPB2
C	668	GLU	-	expression tag	UNP A0A1W6IPB2
C	669	VAL	-	expression tag	UNP A0A1W6IPB2
C	670	LEU	-	expression tag	UNP A0A1W6IPB2
C	671	PHE	-	expression tag	UNP A0A1W6IPB2
C	672	GLN	-	expression tag	UNP A0A1W6IPB2
C	673	GLY	-	expression tag	UNP A0A1W6IPB2
C	674	PRO	-	expression tag	UNP A0A1W6IPB2
C	675	GLY	-	expression tag	UNP A0A1W6IPB2

Continued on next page...

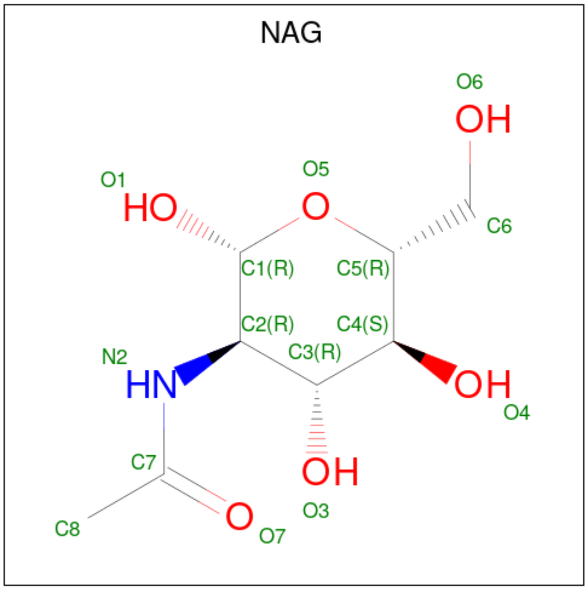
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	676	HIS	-	expression tag	UNP A0A1W6IPB2
C	677	HIS	-	expression tag	UNP A0A1W6IPB2
C	678	HIS	-	expression tag	UNP A0A1W6IPB2
C	679	HIS	-	expression tag	UNP A0A1W6IPB2
C	680	HIS	-	expression tag	UNP A0A1W6IPB2
C	681	HIS	-	expression tag	UNP A0A1W6IPB2
C	682	HIS	-	expression tag	UNP A0A1W6IPB2
C	683	HIS	-	expression tag	UNP A0A1W6IPB2
C	684	SER	-	expression tag	UNP A0A1W6IPB2
C	685	ALA	-	expression tag	UNP A0A1W6IPB2
C	686	TRP	-	expression tag	UNP A0A1W6IPB2
C	687	SER	-	expression tag	UNP A0A1W6IPB2
C	688	HIS	-	expression tag	UNP A0A1W6IPB2
C	689	PRO	-	expression tag	UNP A0A1W6IPB2
C	690	GLN	-	expression tag	UNP A0A1W6IPB2
C	691	PHE	-	expression tag	UNP A0A1W6IPB2
C	692	GLU	-	expression tag	UNP A0A1W6IPB2
C	693	LYS	-	expression tag	UNP A0A1W6IPB2
C	694	GLY	-	expression tag	UNP A0A1W6IPB2
C	695	GLY	-	expression tag	UNP A0A1W6IPB2
C	696	GLY	-	expression tag	UNP A0A1W6IPB2
C	697	SER	-	expression tag	UNP A0A1W6IPB2
C	698	GLY	-	expression tag	UNP A0A1W6IPB2
C	699	GLY	-	expression tag	UNP A0A1W6IPB2
C	700	GLY	-	expression tag	UNP A0A1W6IPB2
C	701	GLY	-	expression tag	UNP A0A1W6IPB2
C	702	SER	-	expression tag	UNP A0A1W6IPB2
C	703	GLY	-	expression tag	UNP A0A1W6IPB2
C	704	GLY	-	expression tag	UNP A0A1W6IPB2
C	705	SER	-	expression tag	UNP A0A1W6IPB2
C	706	ALA	-	expression tag	UNP A0A1W6IPB2
C	707	TRP	-	expression tag	UNP A0A1W6IPB2
C	708	SER	-	expression tag	UNP A0A1W6IPB2
C	709	HIS	-	expression tag	UNP A0A1W6IPB2
C	710	PRO	-	expression tag	UNP A0A1W6IPB2
C	711	GLN	-	expression tag	UNP A0A1W6IPB2
C	712	PHE	-	expression tag	UNP A0A1W6IPB2
C	713	GLU	-	expression tag	UNP A0A1W6IPB2
C	714	LYS	-	expression tag	UNP A0A1W6IPB2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

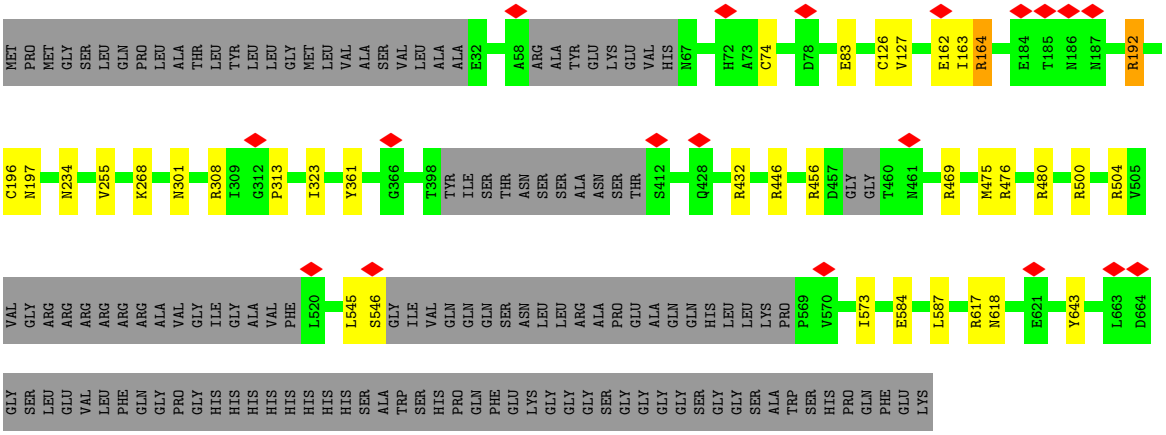
Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total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

3 Residue-property plots (i)

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

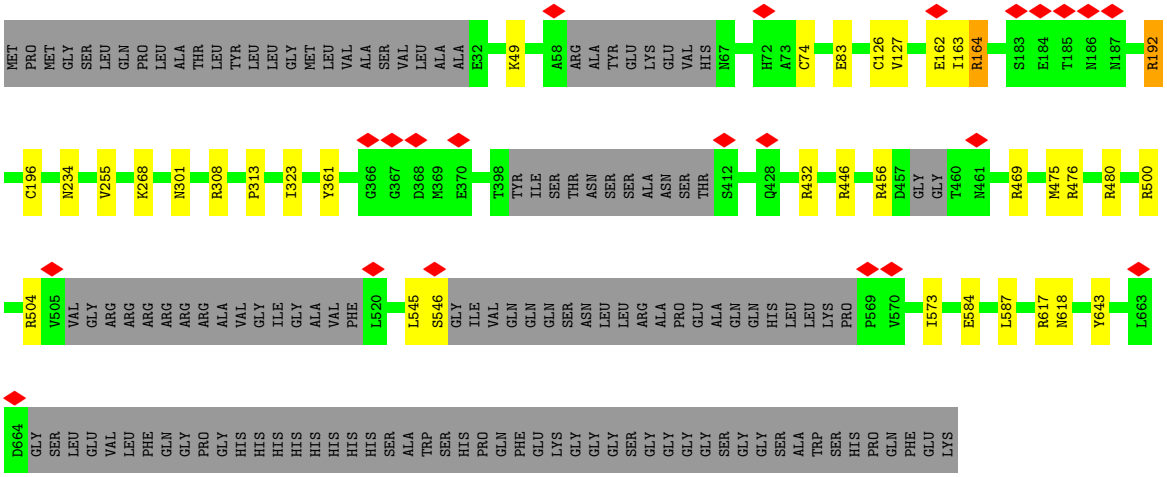
• Molecule 1: CH848 10.17DT SOSIP Envelope glycoprotein gp160

Chain A:



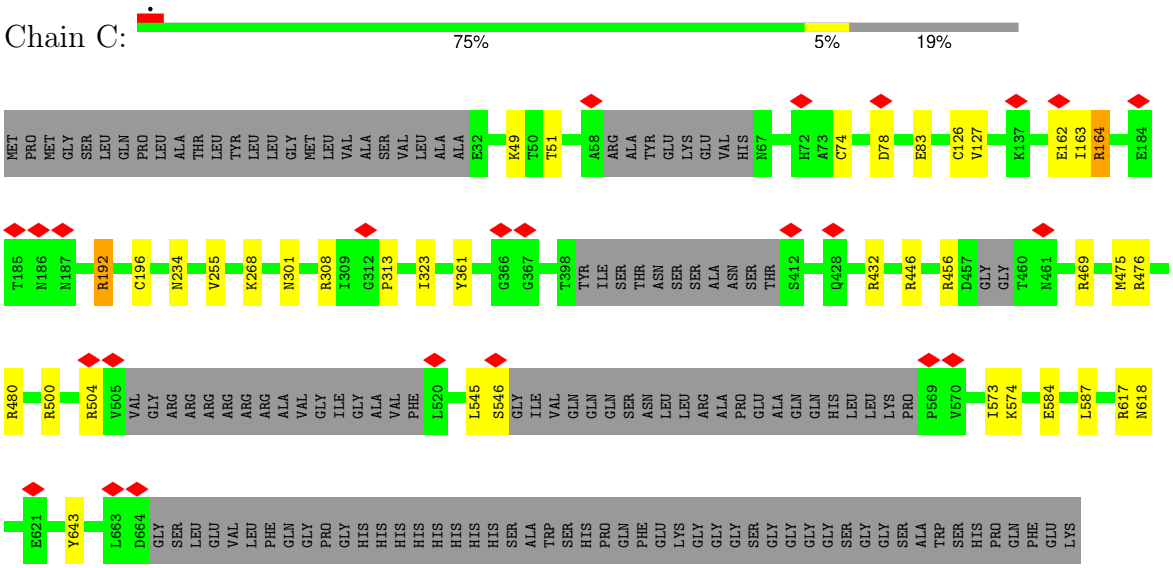
• Molecule 1: CH848 10.17DT SOSIP Envelope glycoprotein gp160

Chain B:



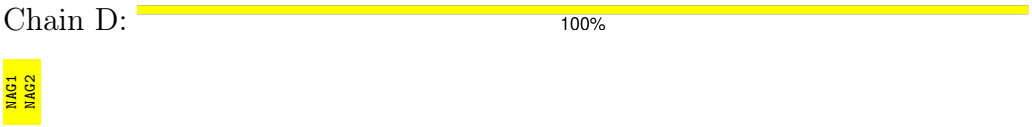
• Molecule 1: CH848 10.17DT SOSIP Envelope glycoprotein gp160

Chain C:



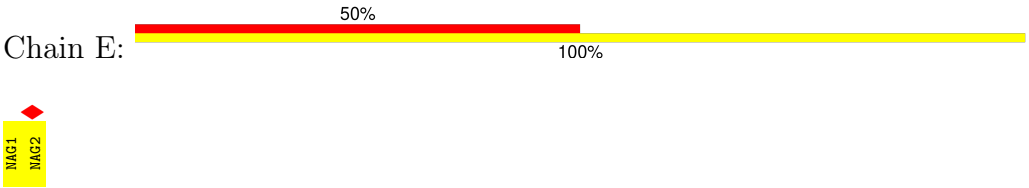
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



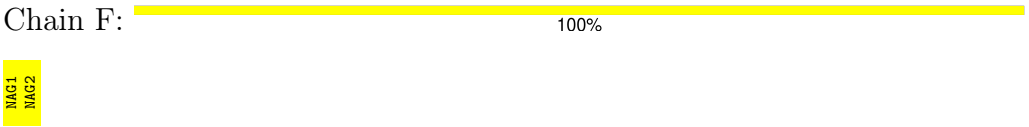
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



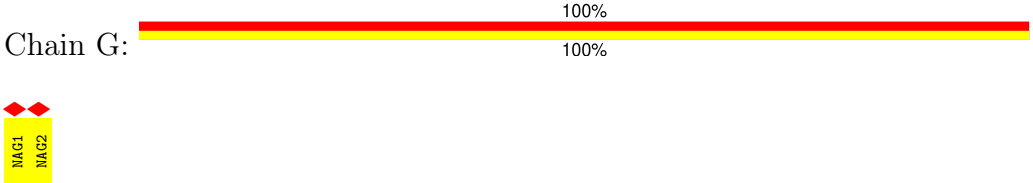
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



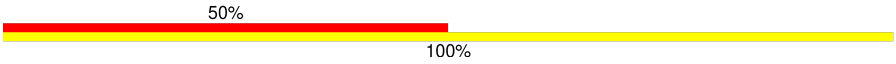
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



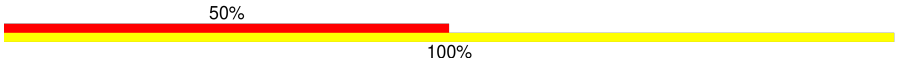
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



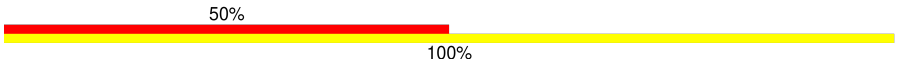
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



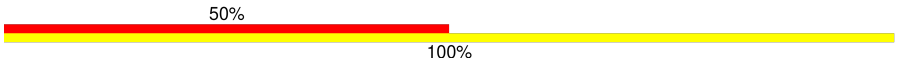
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



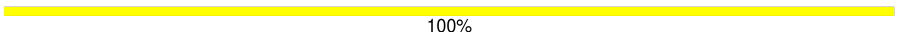
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



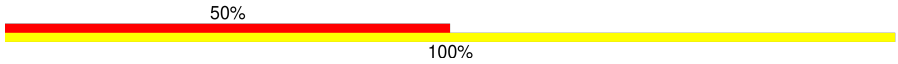
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



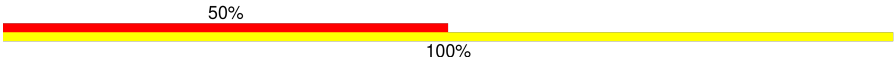
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



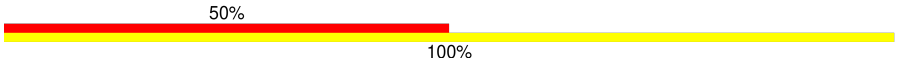
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



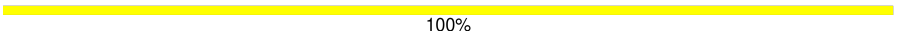
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



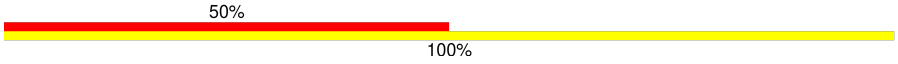
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



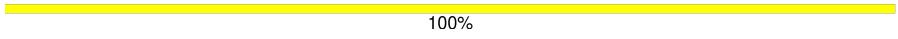
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:

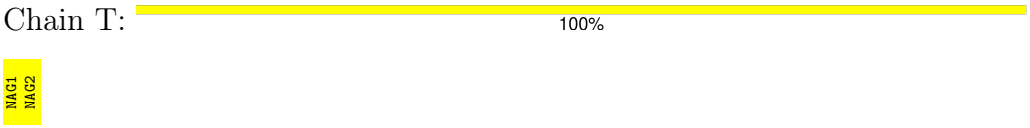


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

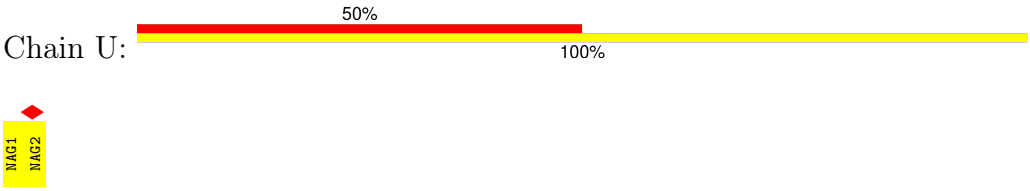
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	111026	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 ($e^-/Å^2$)	61	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.011	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.60	0/4522	0.97	11/6145 (0.2%)
1	B	0.60	0/4522	0.97	11/6145 (0.2%)
1	C	0.60	0/4522	0.97	11/6145 (0.2%)
All	All	0.60	0/13566	0.97	33/18435 (0.2%)

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

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

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	476	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	C	476	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	476	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	500	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	500	ARG	NE-CZ-NH2	7.02	123.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	TYR	Sidechain
1	B	361	TYR	Sidechain
1	C	361	TYR	Sidechain

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	4433	0	4328	45	0
1	B	4433	0	4328	46	0
1	C	4433	0	4328	47	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
3	A	126	0	117	5	0
3	B	126	0	117	5	0
3	C	126	0	117	5	0
All	All	14181	0	13785	92	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 3.

The worst 5 of 92 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:C:618:ASN:ND2	3:C:809:NAG:C1	1.70	1.54
1:B:618:ASN:ND2	3:B:809:NAG:C1	1.70	1.52
1:A:618:ASN:ND2	3:A:809:NAG:C1	1.70	1.51
1:A:162:GLU:CB	1:C:196:CYS:O	1.76	1.34
1:B:196:CYS:O	1:C:162:GLU:CB	1.76	1.33

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	552/698 (79%)	522 (95%)	30 (5%)	0	100	100
1	B	552/698 (79%)	522 (95%)	30 (5%)	0	100	100
1	C	552/698 (79%)	522 (95%)	30 (5%)	0	100	100
All	All	1656/2094 (79%)	1566 (95%)	90 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	500/602 (83%)	495 (99%)	5 (1%)	73	82
1	B	500/602 (83%)	494 (99%)	6 (1%)	67	79
1	C	500/602 (83%)	493 (99%)	7 (1%)	62	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1500/1806 (83%)	1482 (99%)	18 (1%)	66 79

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	83	GLU
1	C	504	ARG
1	C	268	LYS
1	B	234	ASN
1	C	78	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	374	HIS

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)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	0.86	1 (5%)
2	NAG	D	2	2	14,14,15	1.24	2 (14%)	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	1	1,2	14,14,15	1.23	2 (14%)	17,19,21	0.78	0
2	NAG	E	2	2	14,14,15	1.31	3 (21%)	17,19,21	1.15	2 (11%)
2	NAG	F	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	0.98	1 (5%)
2	NAG	F	2	2	14,14,15	1.12	1 (7%)	17,19,21	0.71	0
2	NAG	G	1	1,2	14,14,15	1.32	2 (14%)	17,19,21	0.99	1 (5%)
2	NAG	G	2	2	14,14,15	1.34	3 (21%)	17,19,21	0.95	1 (5%)
2	NAG	H	1	1,2	14,14,15	1.26	2 (14%)	17,19,21	0.72	0
2	NAG	H	2	2	14,14,15	1.33	2 (14%)	17,19,21	1.16	1 (5%)
2	NAG	I	1	1,2	14,14,15	1.40	3 (21%)	17,19,21	0.87	1 (5%)
2	NAG	I	2	2	14,14,15	1.28	1 (7%)	17,19,21	0.93	1 (5%)
2	NAG	J	1	1,2	14,14,15	1.15	1 (7%)	17,19,21	0.86	1 (5%)
2	NAG	J	2	2	14,14,15	1.24	2 (14%)	17,19,21	0.74	0
2	NAG	K	1	1,2	14,14,15	1.23	2 (14%)	17,19,21	0.78	0
2	NAG	K	2	2	14,14,15	1.30	3 (21%)	17,19,21	1.15	2 (11%)
2	NAG	L	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	L	2	2	14,14,15	1.14	1 (7%)	17,19,21	0.71	0
2	NAG	M	1	1,2	14,14,15	1.33	2 (14%)	17,19,21	0.99	1 (5%)
2	NAG	M	2	2	14,14,15	1.34	3 (21%)	17,19,21	0.95	1 (5%)
2	NAG	N	1	1,2	14,14,15	1.26	3 (21%)	17,19,21	0.72	0
2	NAG	N	2	2	14,14,15	1.32	1 (7%)	17,19,21	1.16	1 (5%)
2	NAG	O	1	1,2	14,14,15	1.40	3 (21%)	17,19,21	0.87	1 (5%)
2	NAG	O	2	2	14,14,15	1.28	1 (7%)	17,19,21	0.93	1 (5%)
2	NAG	P	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	0.85	1 (5%)
2	NAG	P	2	2	14,14,15	1.24	2 (14%)	17,19,21	0.74	0
2	NAG	Q	1	1,2	14,14,15	1.23	2 (14%)	17,19,21	0.78	0
2	NAG	Q	2	2	14,14,15	1.31	3 (21%)	17,19,21	1.14	2 (11%)
2	NAG	R	1	1,2	14,14,15	1.03	1 (7%)	17,19,21	0.98	1 (5%)
2	NAG	R	2	2	14,14,15	1.13	1 (7%)	17,19,21	0.71	0
2	NAG	S	1	1,2	14,14,15	1.32	2 (14%)	17,19,21	0.99	1 (5%)
2	NAG	S	2	2	14,14,15	1.34	3 (21%)	17,19,21	0.95	1 (5%)
2	NAG	T	1	1,2	14,14,15	1.25	2 (14%)	17,19,21	0.72	0
2	NAG	T	2	2	14,14,15	1.33	1 (7%)	17,19,21	1.16	1 (5%)
2	NAG	U	1	1,2	14,14,15	1.40	3 (21%)	17,19,21	0.87	1 (5%)
2	NAG	U	2	2	14,14,15	1.27	1 (7%)	17,19,21	0.93	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	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	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	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	O5-C5	3.01	1.49	1.43
2	T	2	NAG	O5-C5	2.99	1.49	1.43
2	N	2	NAG	O5-C5	2.98	1.49	1.43
2	G	2	NAG	O5-C5	2.95	1.49	1.43
2	M	2	NAG	O5-C5	2.95	1.49	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C1-O5-C5	3.05	116.27	112.19
2	U	2	NAG	C1-O5-C5	3.04	116.26	112.19
2	O	2	NAG	C1-O5-C5	3.03	116.25	112.19
2	N	2	NAG	C1-O5-C5	2.84	115.99	112.19
2	T	2	NAG	C1-O5-C5	2.83	115.98	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

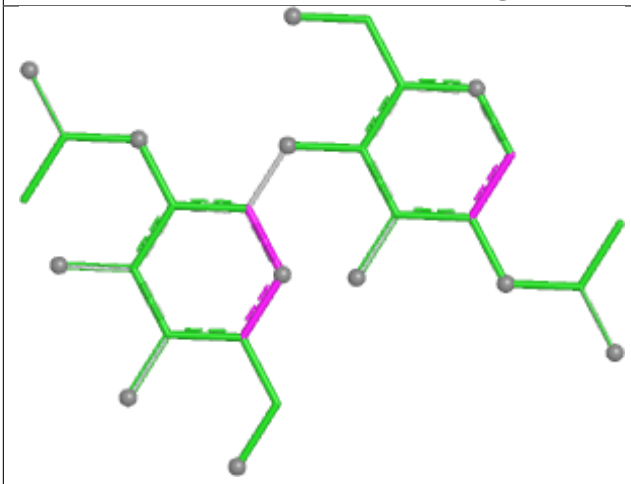
Mol	Chain	Res	Type	Atoms
2	M	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

There are no ring outliers.

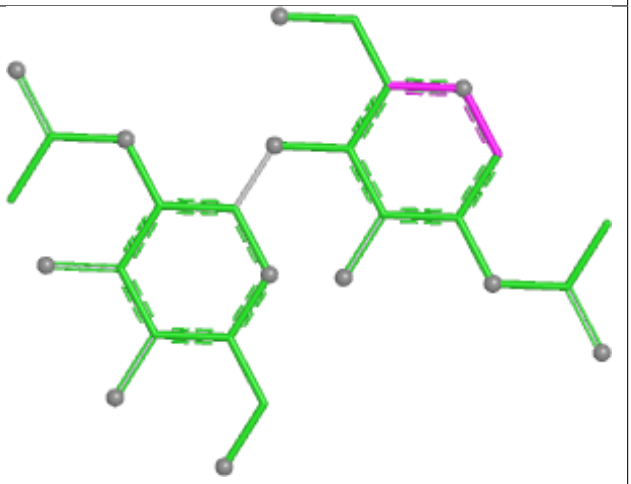
No monomer is involved in short contacts.

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

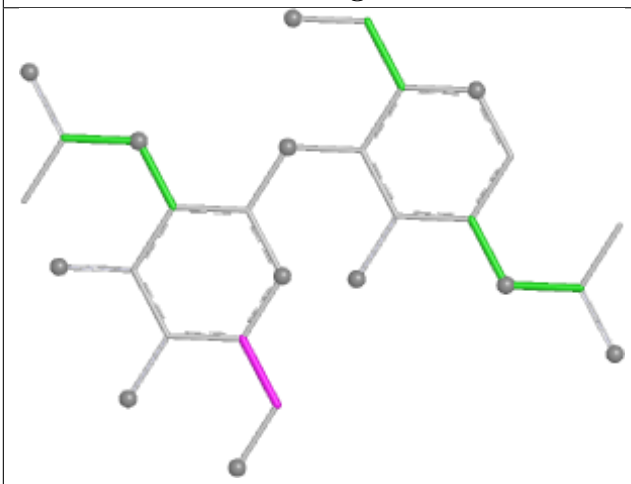
Oligosaccharide Chain D



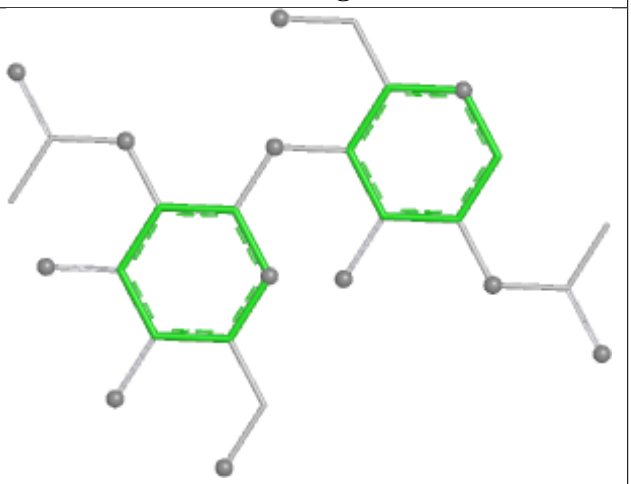
Bond lengths



Bond angles

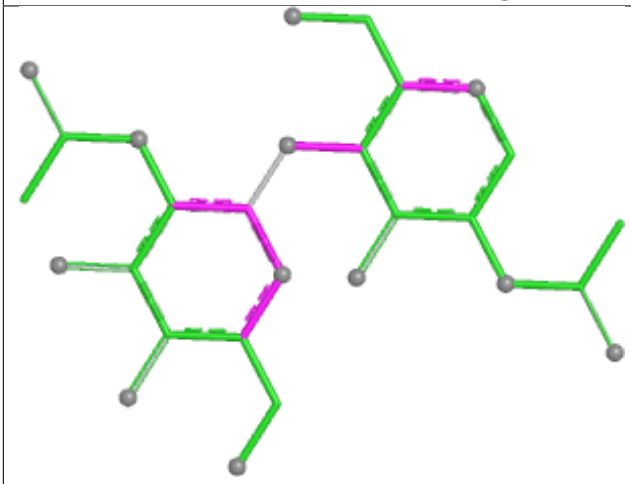


Torsions

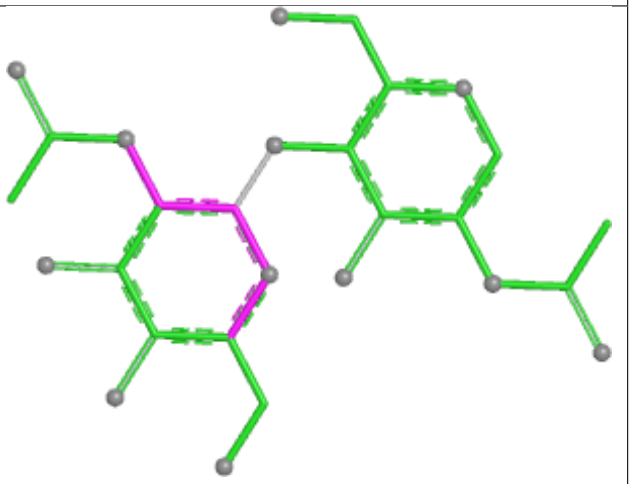


Rings

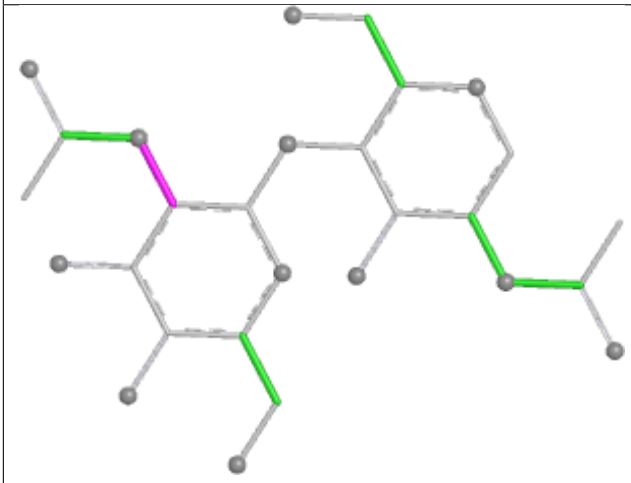
Oligosaccharide Chain E



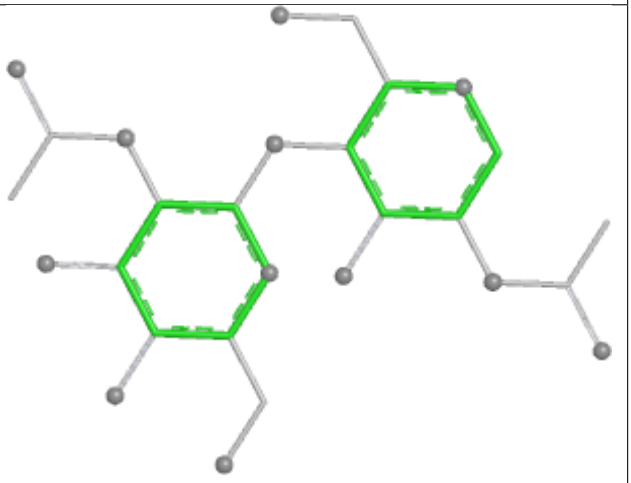
Bond lengths



Bond angles

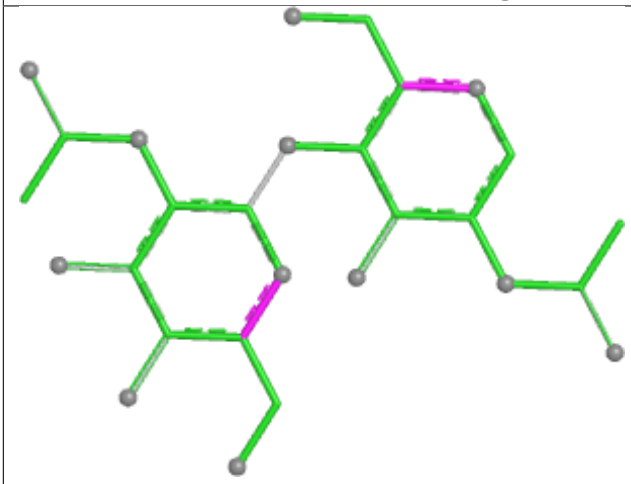


Torsions

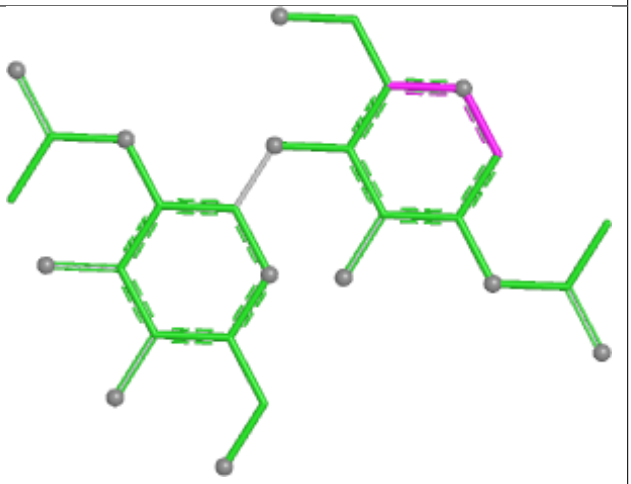


Rings

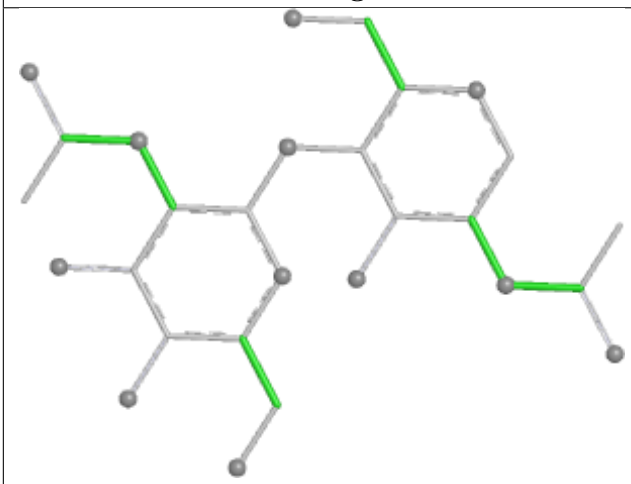
Oligosaccharide Chain F



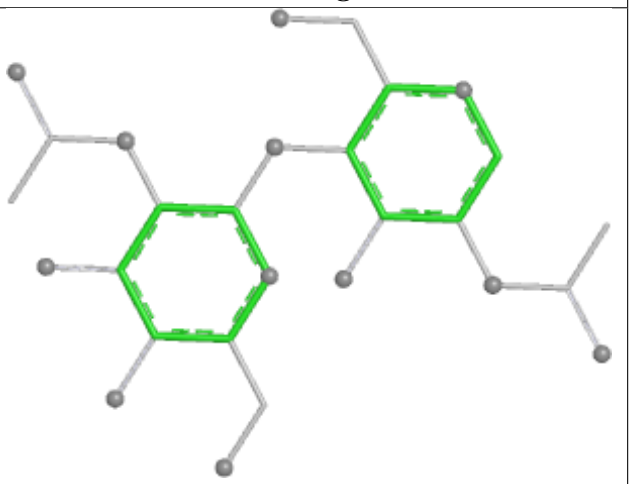
Bond lengths



Bond angles

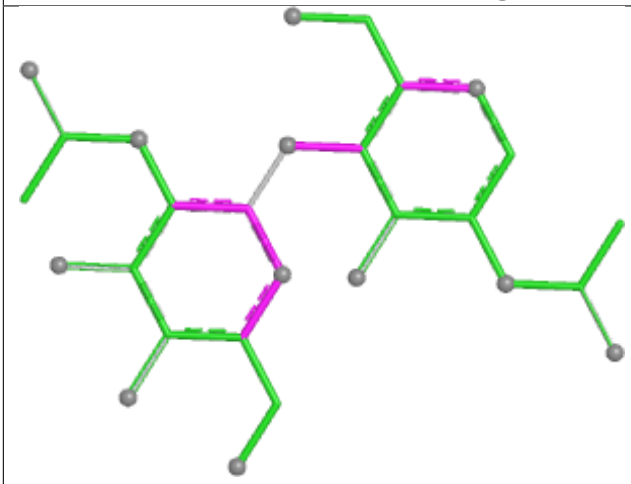


Torsions

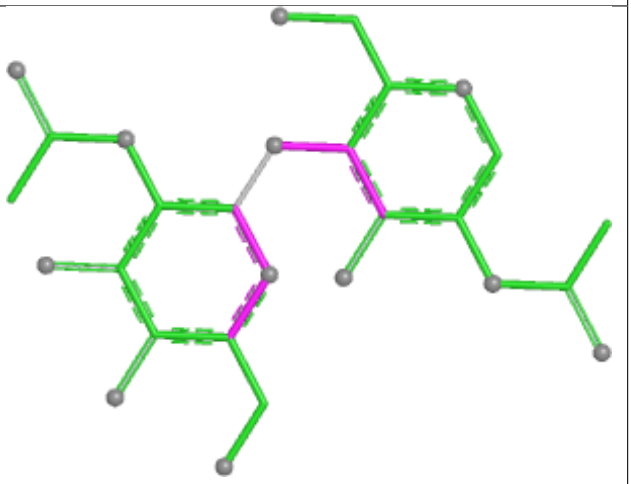


Rings

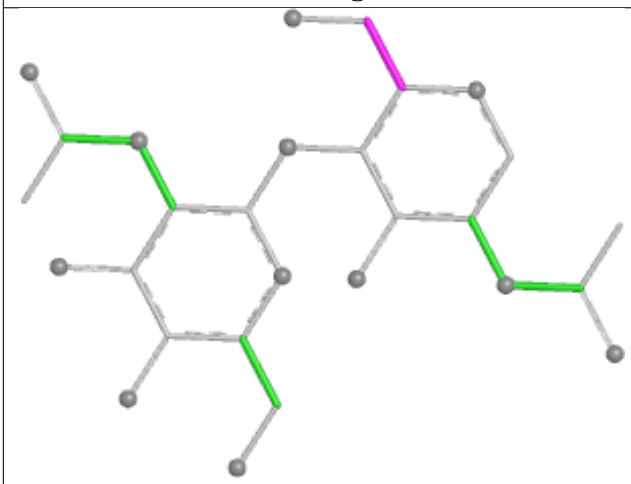
Oligosaccharide Chain G



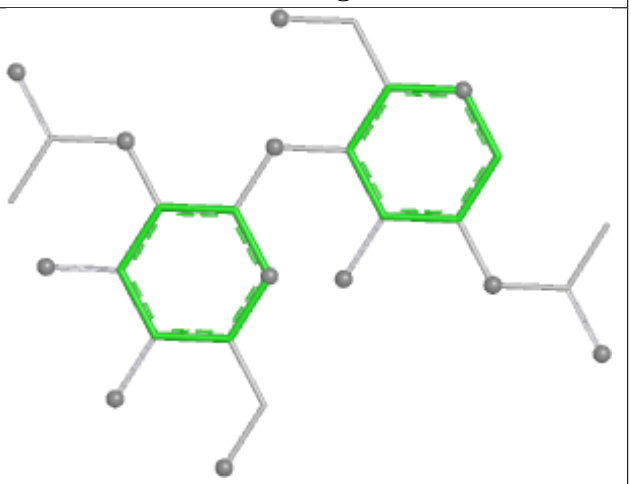
Bond lengths



Bond angles

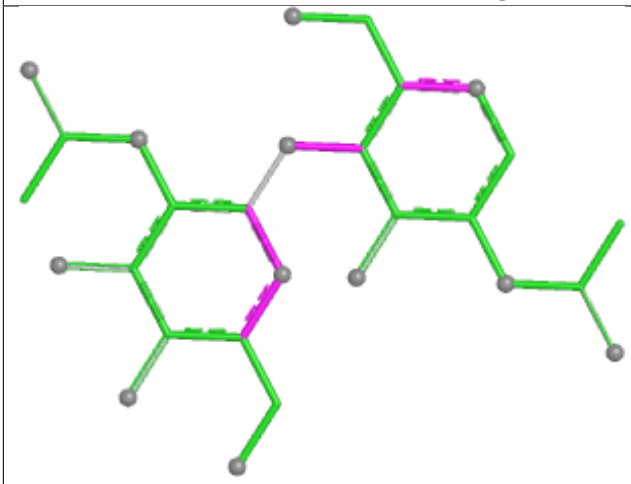


Torsions

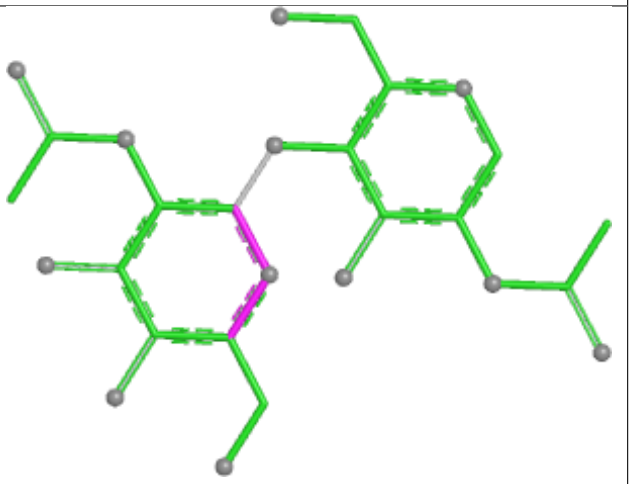


Rings

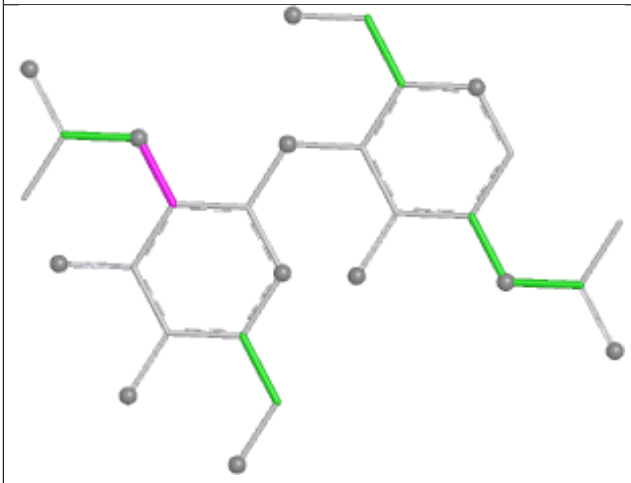
Oligosaccharide Chain H



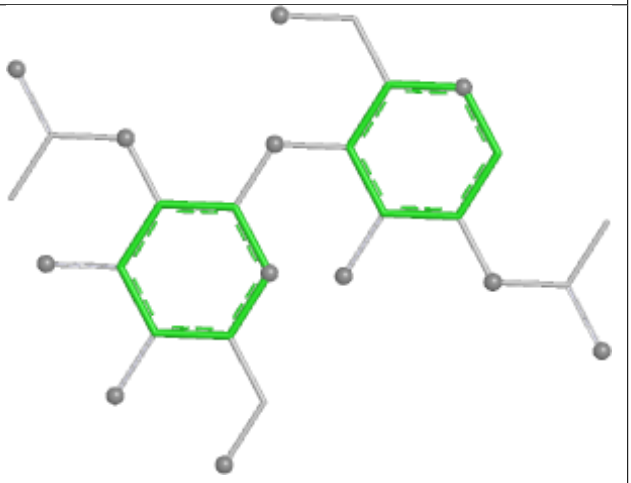
Bond lengths



Bond angles

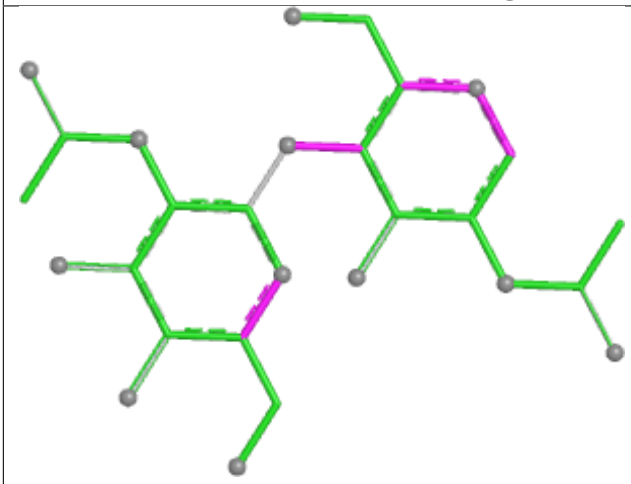


Torsions

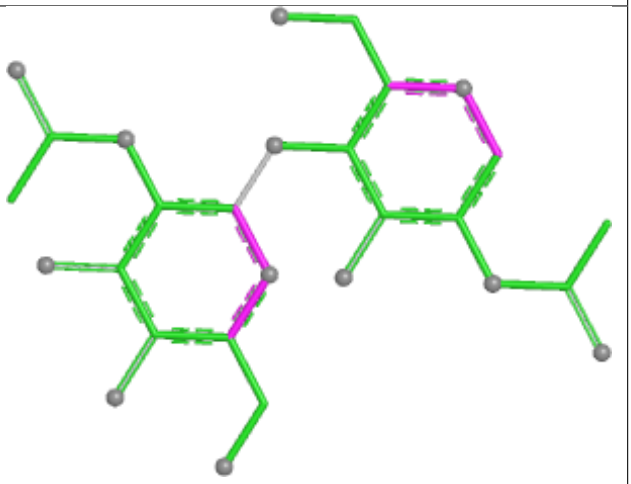


Rings

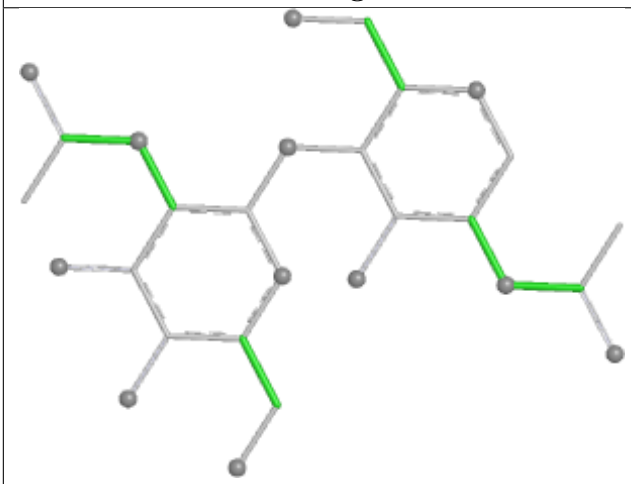
Oligosaccharide Chain I



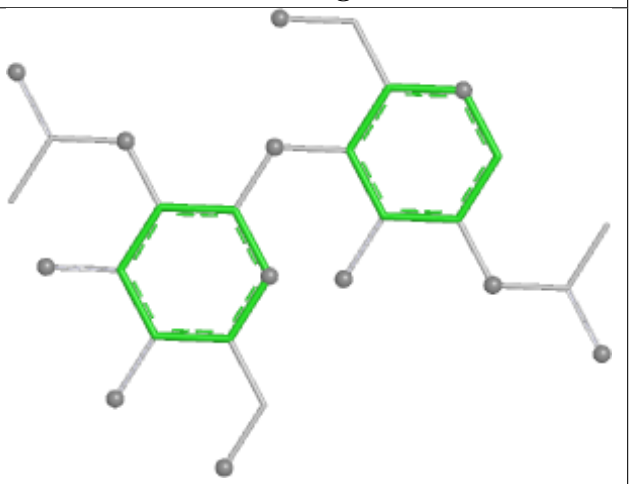
Bond lengths



Bond angles

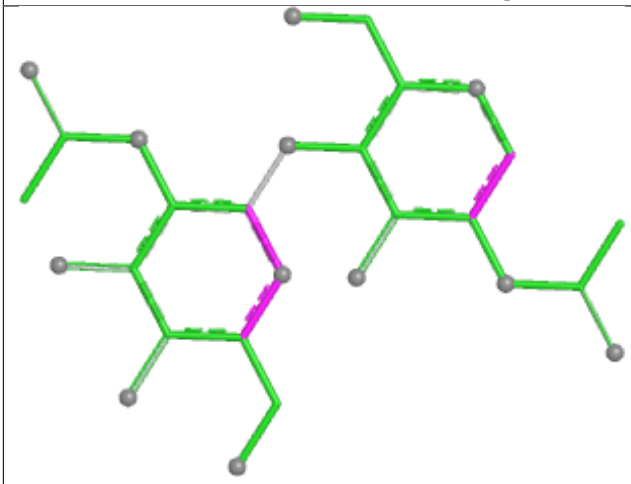


Torsions

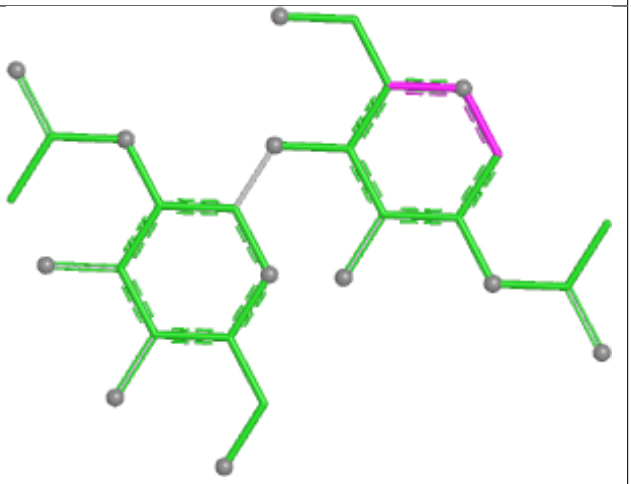


Rings

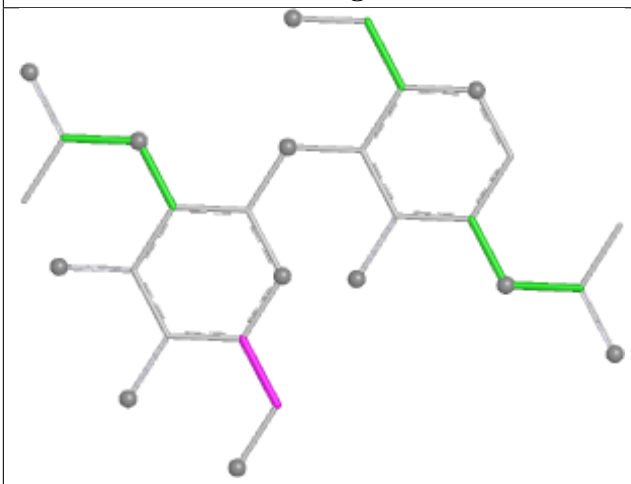
Oligosaccharide Chain J



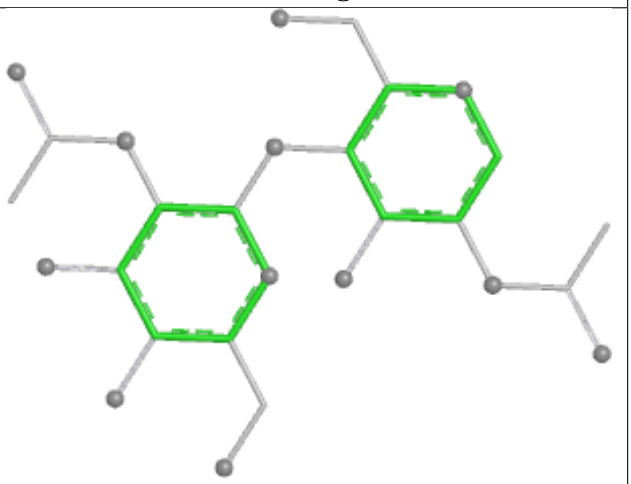
Bond lengths



Bond angles

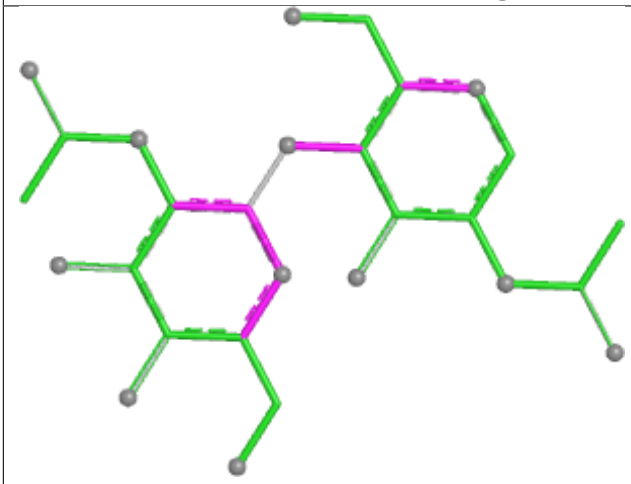


Torsions

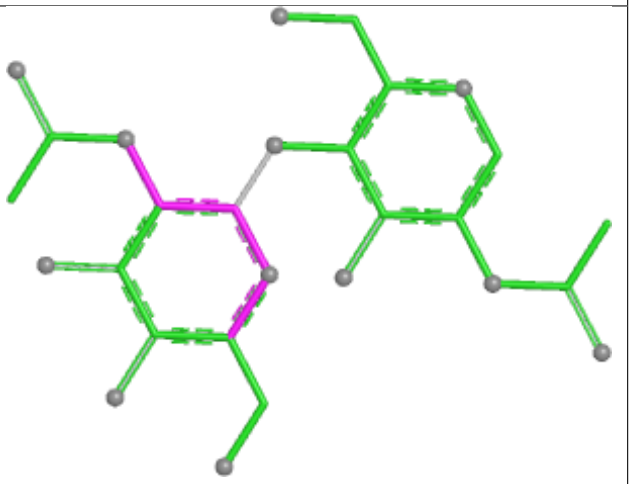


Rings

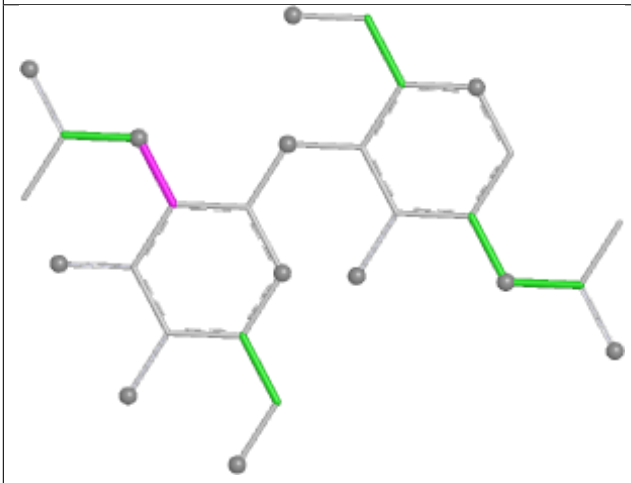
Oligosaccharide Chain K



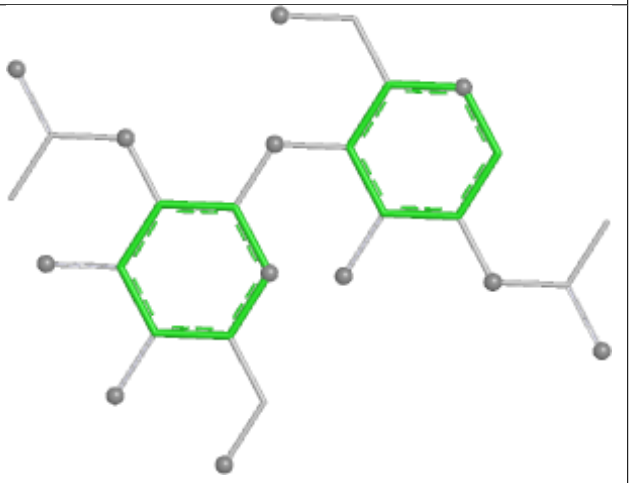
Bond lengths



Bond angles

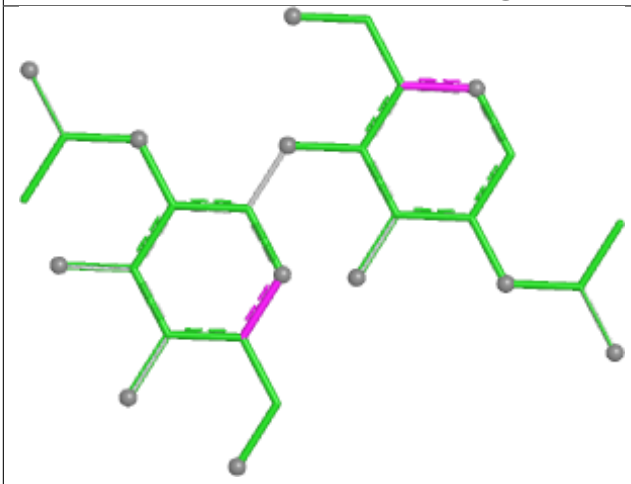


Torsions

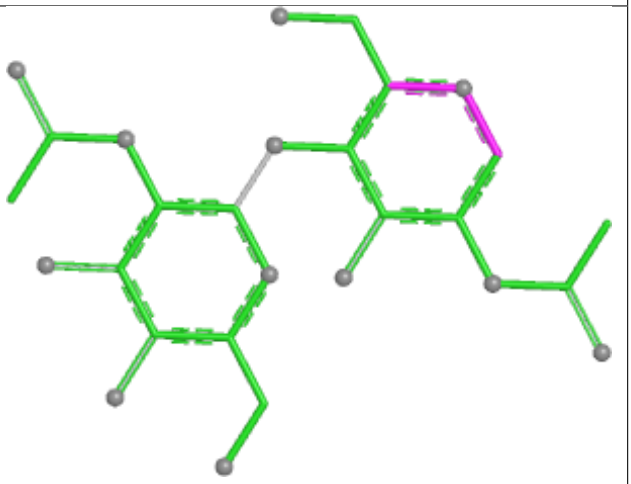


Rings

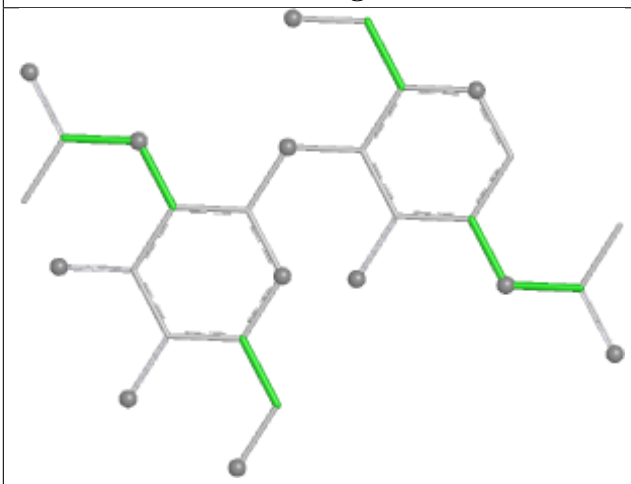
Oligosaccharide Chain L



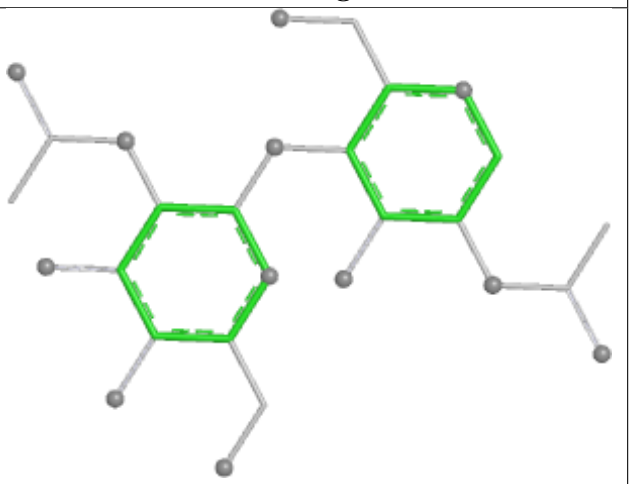
Bond lengths



Bond angles

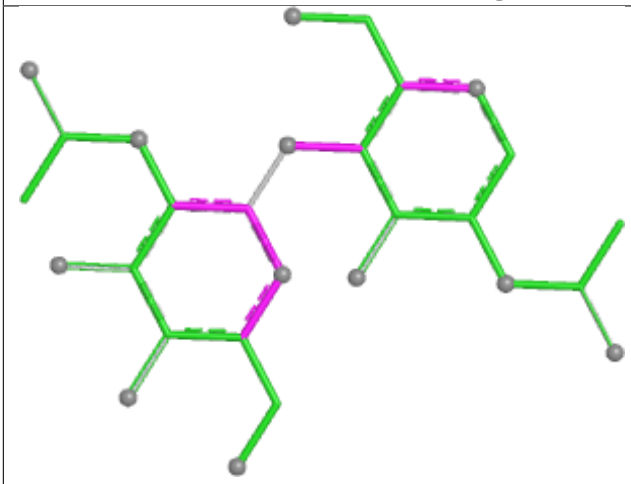


Torsions

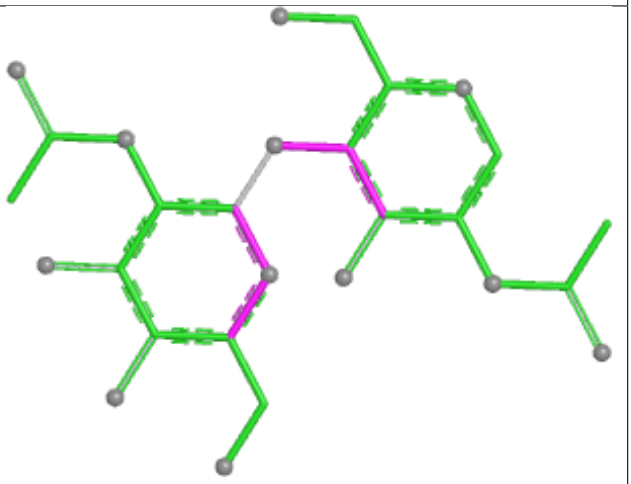


Rings

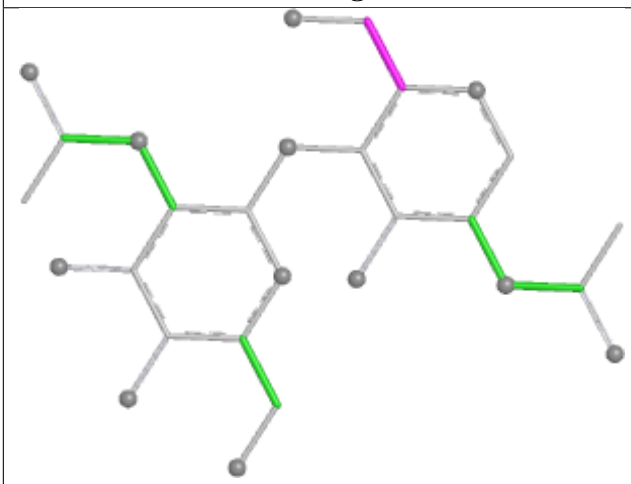
Oligosaccharide Chain M



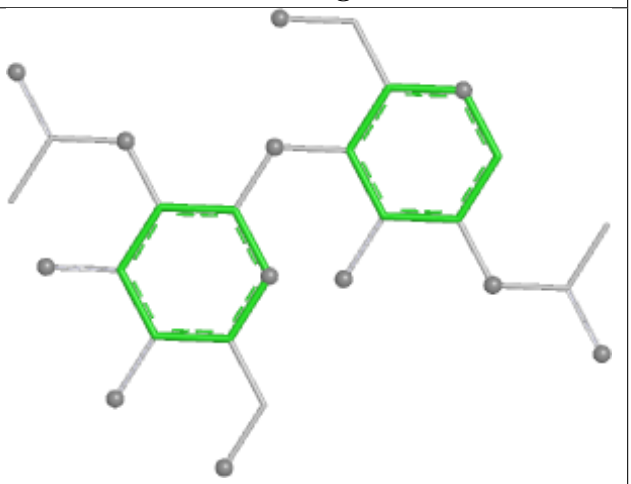
Bond lengths



Bond angles

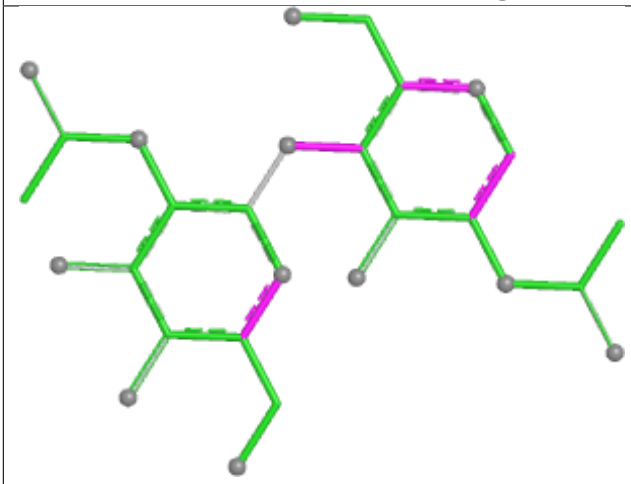


Torsions

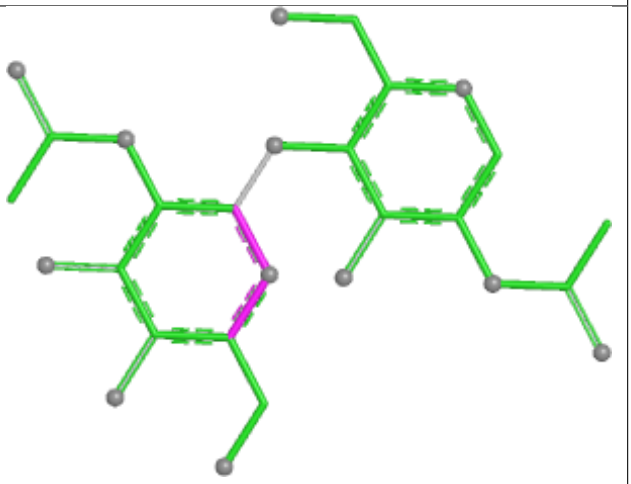


Rings

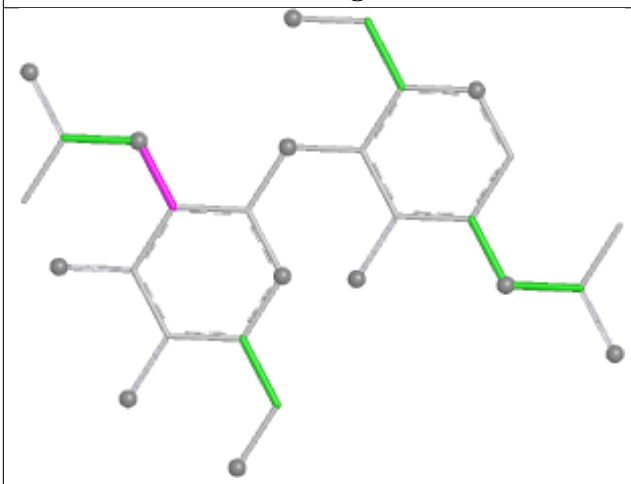
Oligosaccharide Chain N



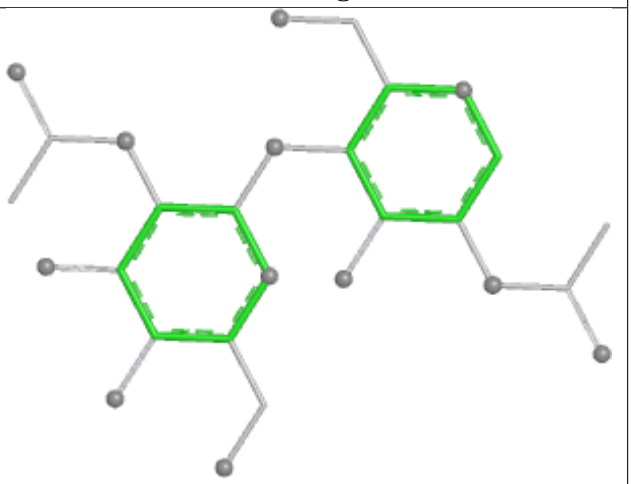
Bond lengths



Bond angles

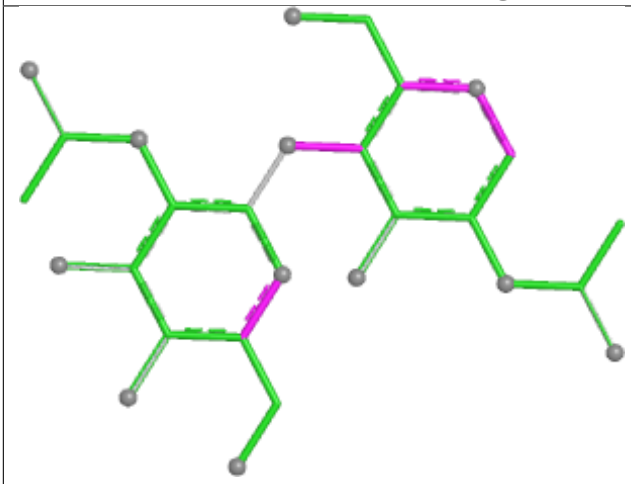


Torsions

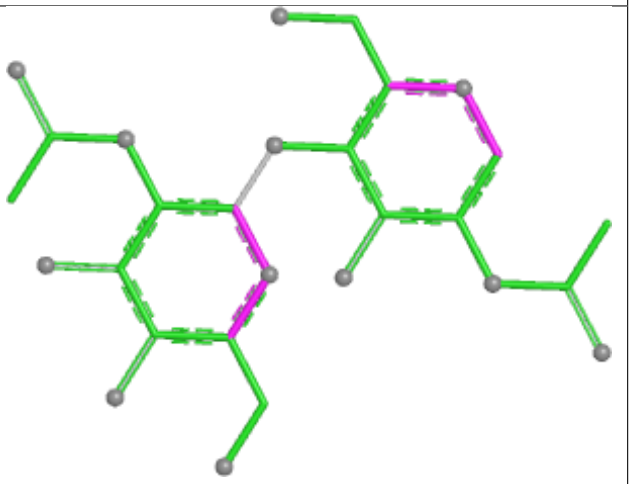


Rings

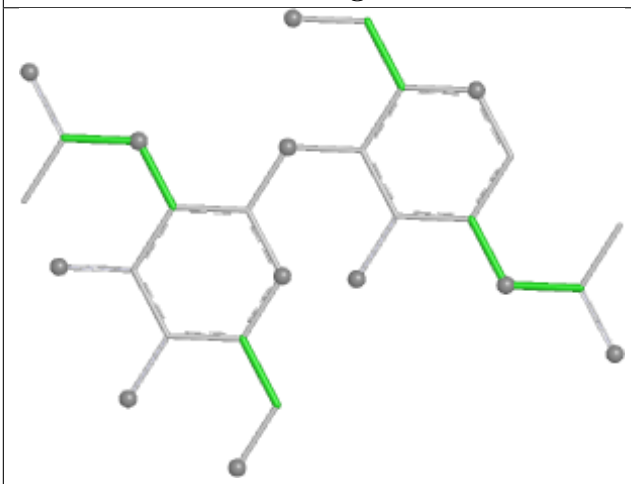
Oligosaccharide Chain O



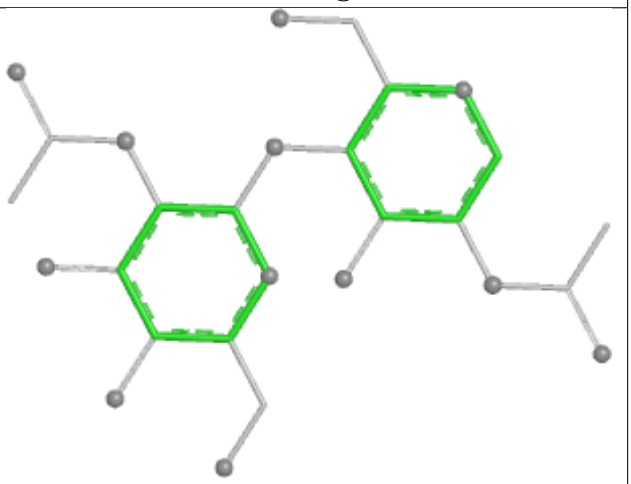
Bond lengths



Bond angles

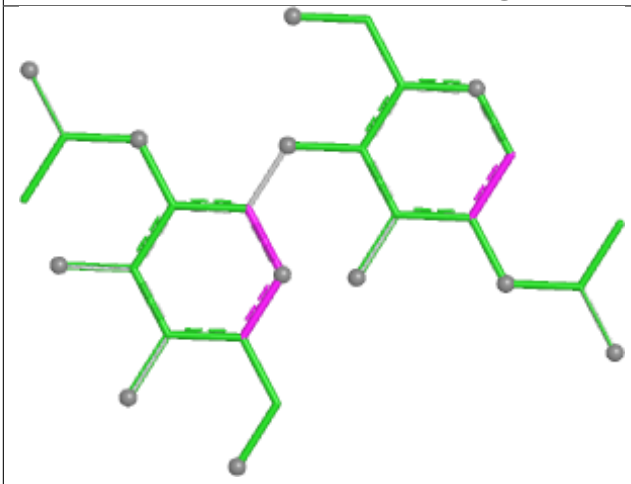


Torsions

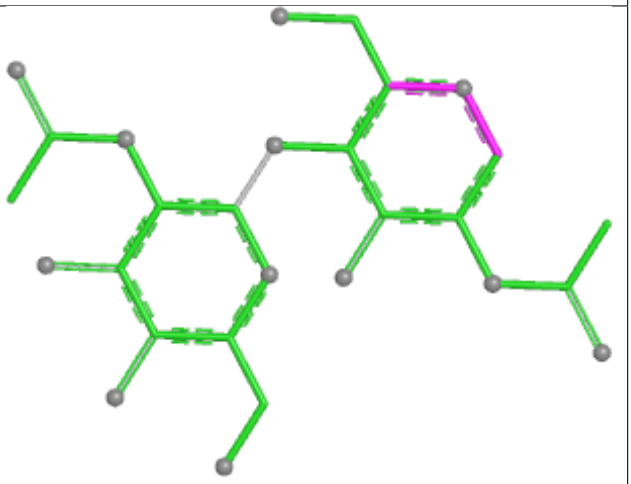


Rings

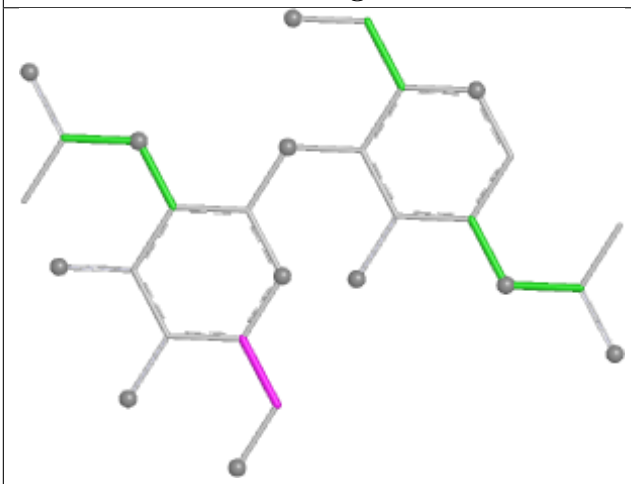
Oligosaccharide Chain P



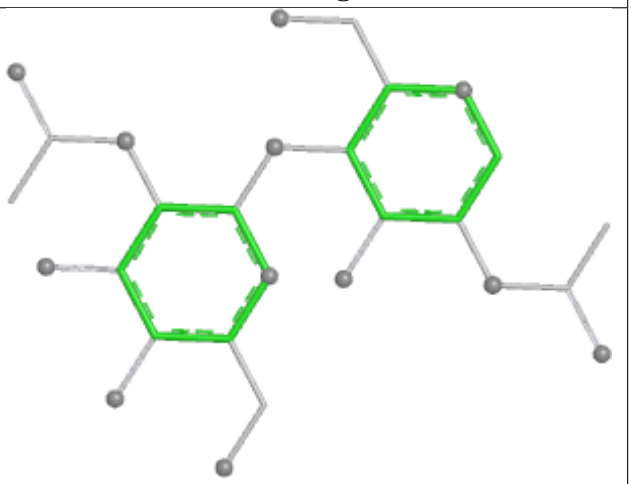
Bond lengths



Bond angles

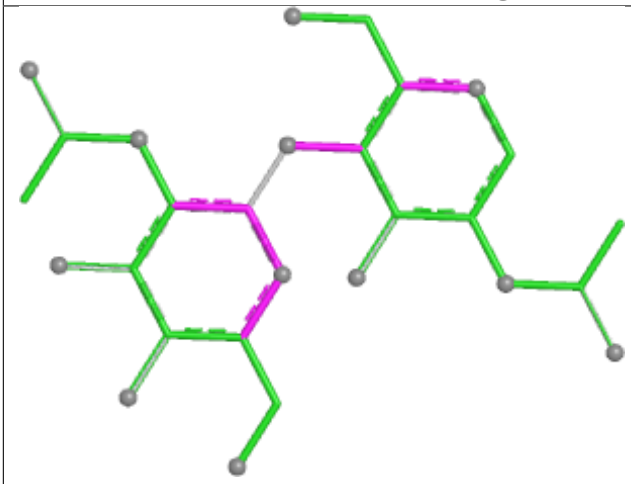


Torsions

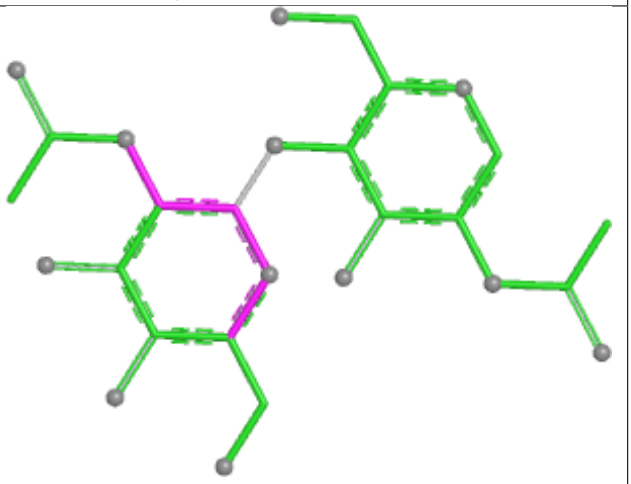


Rings

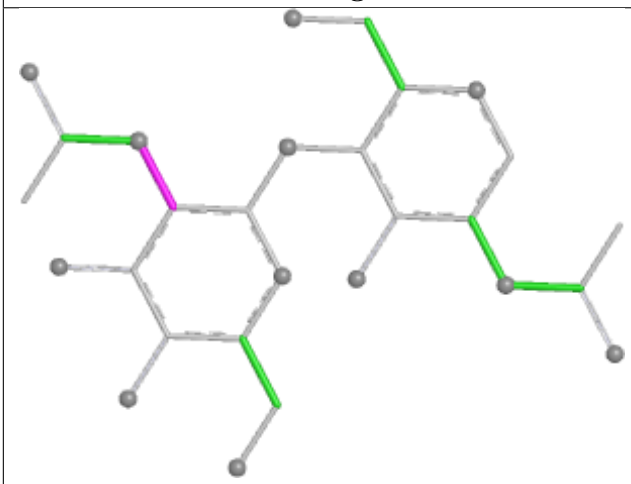
Oligosaccharide Chain Q



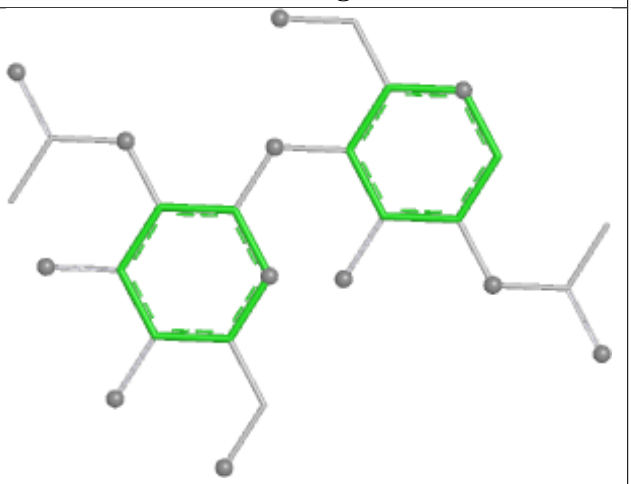
Bond lengths



Bond angles

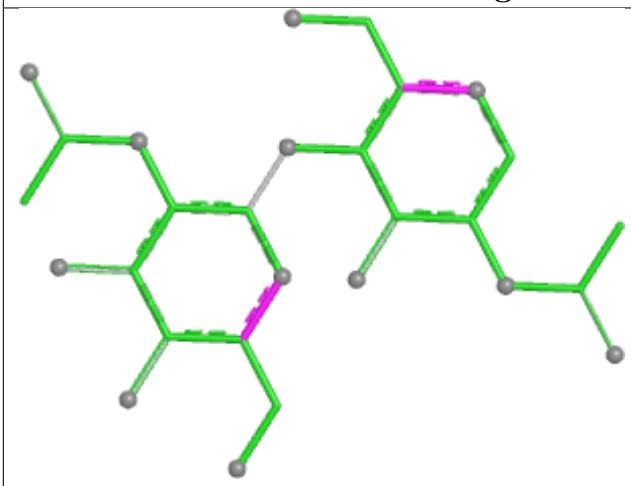


Torsions

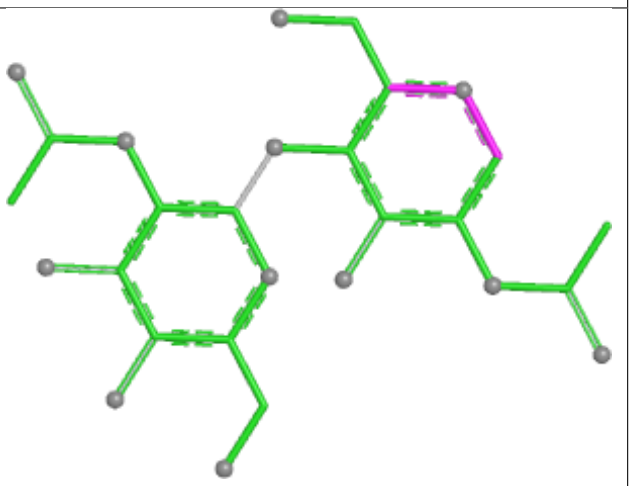


Rings

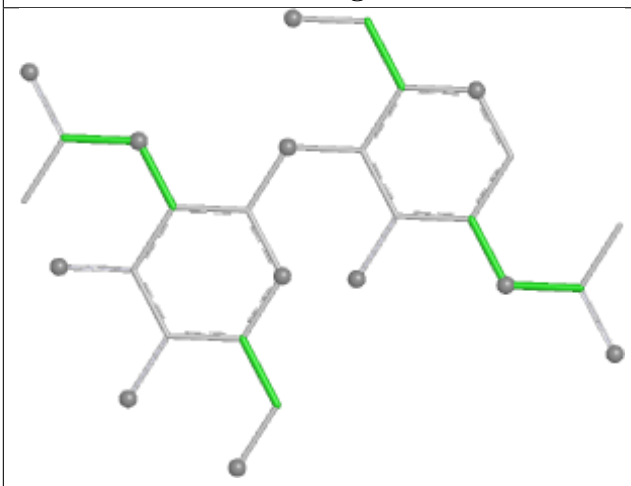
Oligosaccharide Chain R



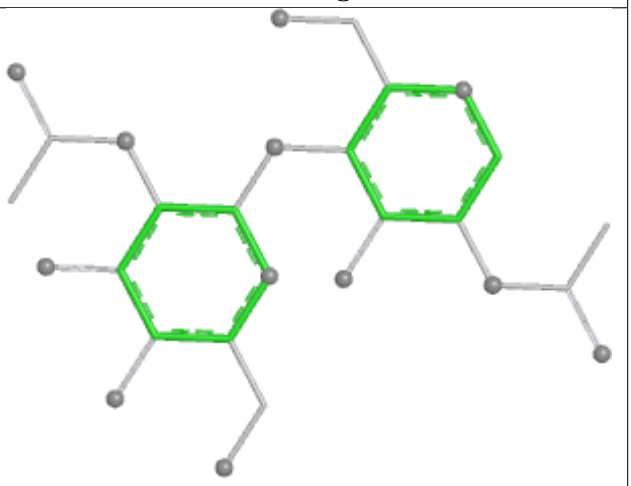
Bond lengths



Bond angles

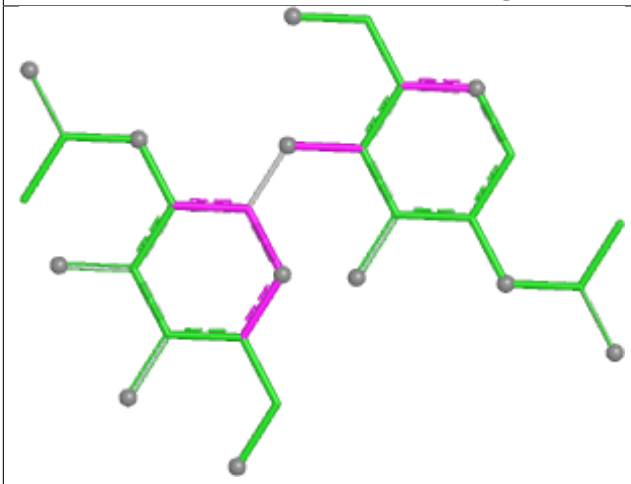


Torsions

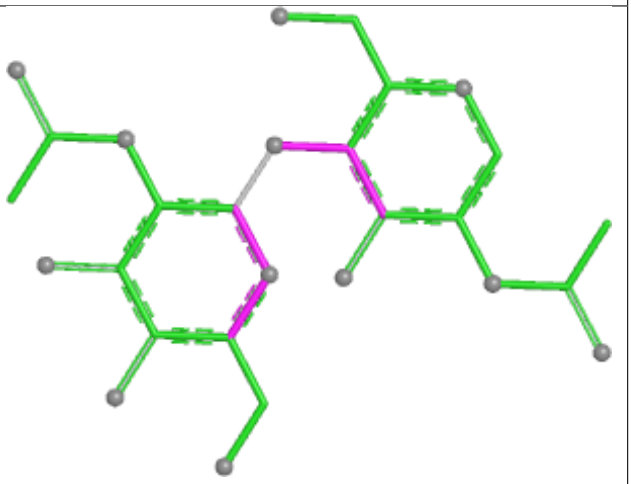


Rings

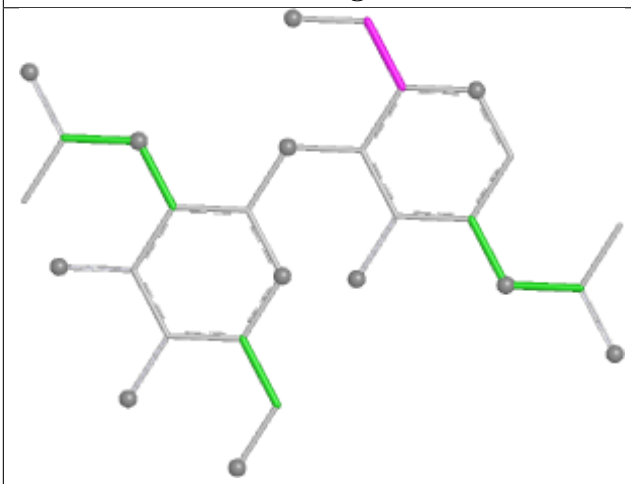
Oligosaccharide Chain S



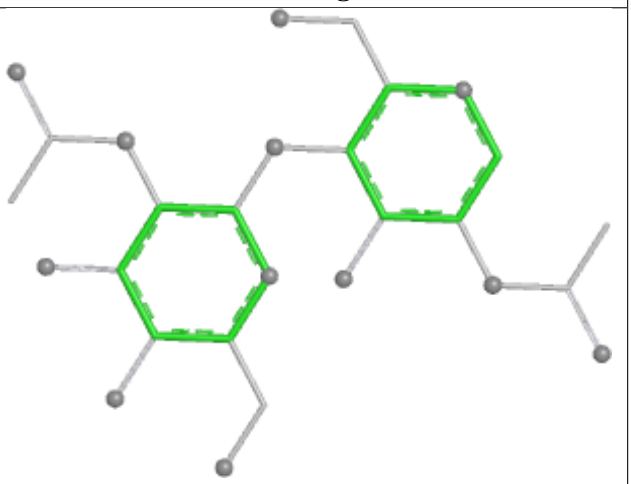
Bond lengths



Bond angles

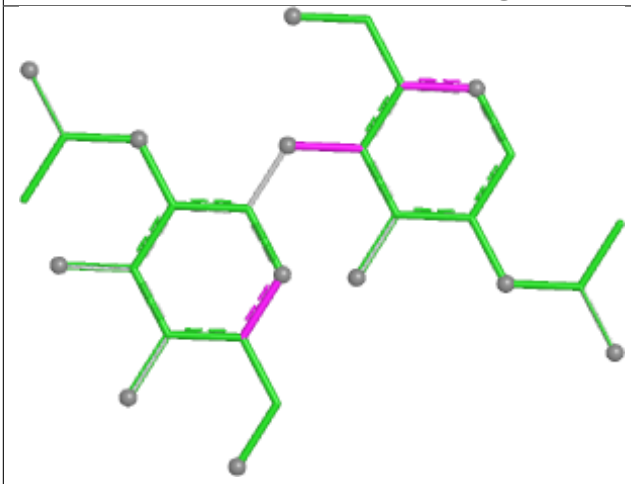


Torsions

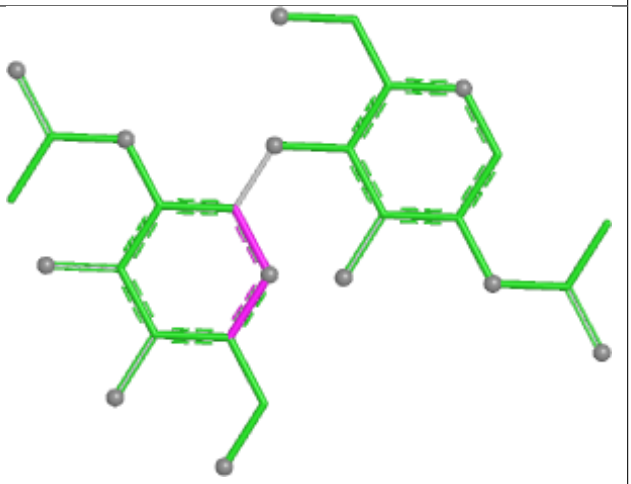


Rings

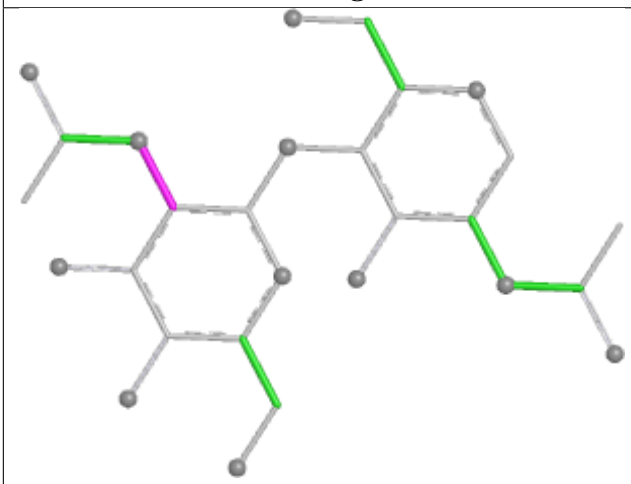
Oligosaccharide Chain T



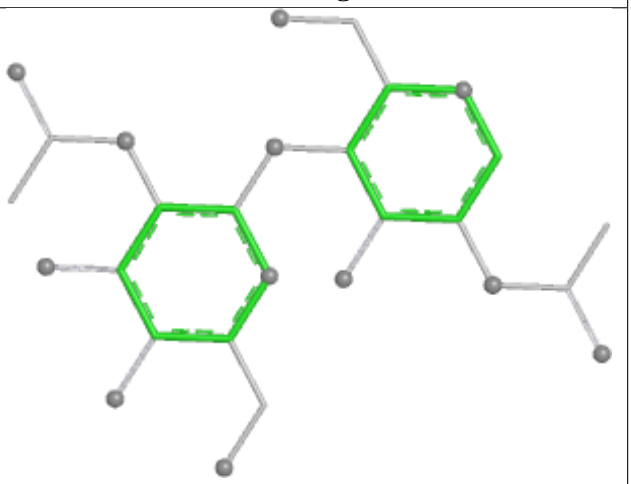
Bond lengths



Bond angles

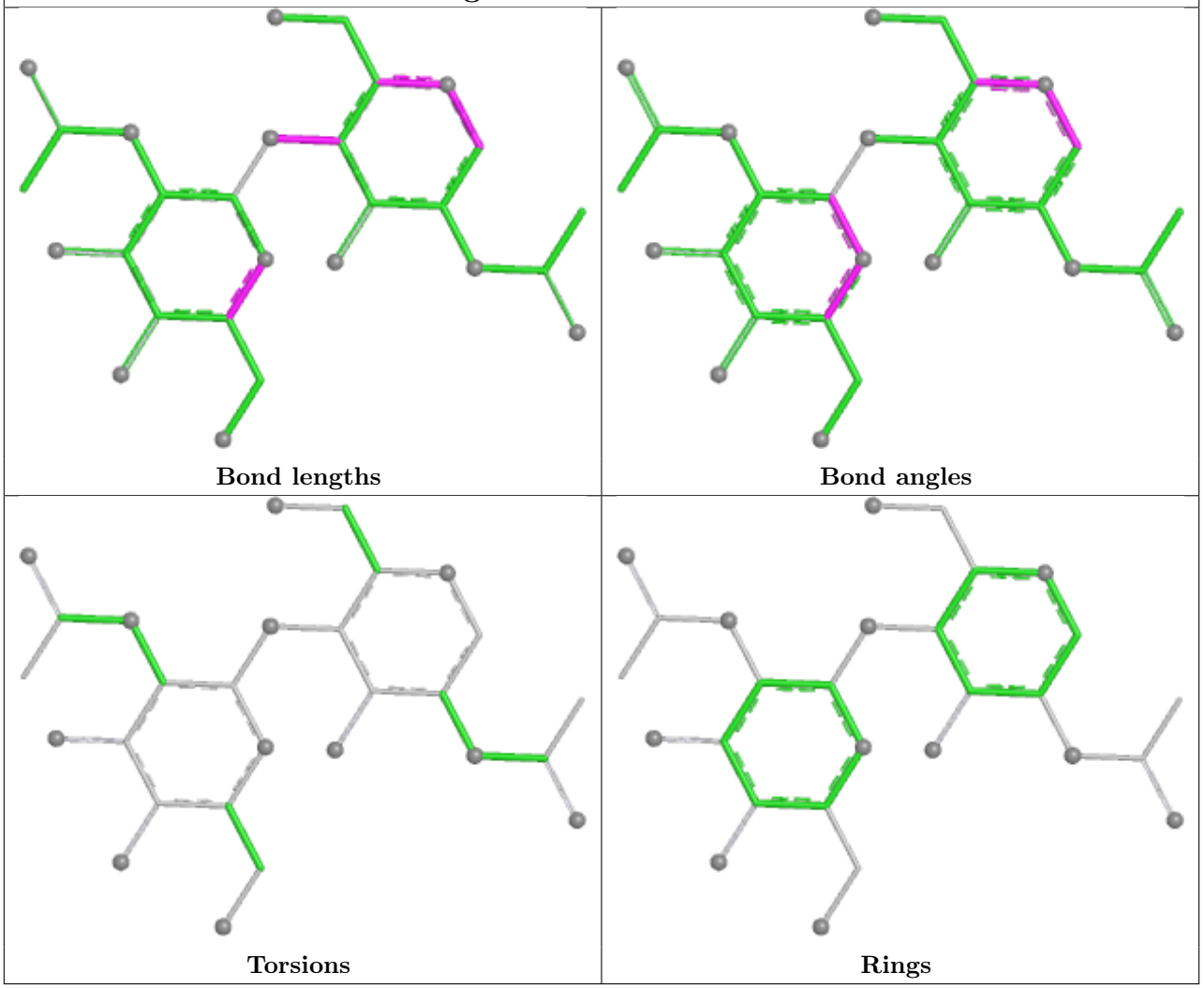


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	NAG	C	801	1	14,14,15	1.29	3 (21%)	17,19,21	0.88	1 (5%)
3	NAG	A	809	-	14,14,15	1.39	3 (21%)	17,19,21	1.10	1 (5%)
3	NAG	B	801	1	14,14,15	1.28	3 (21%)	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	801	1	14,14,15	1.28	3 (21%)	17,19,21	0.89	1 (5%)
3	NAG	C	808	1	14,14,15	1.23	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	C	805	1	14,14,15	1.21	1 (7%)	17,19,21	0.61	0
3	NAG	B	809	-	14,14,15	1.40	3 (21%)	17,19,21	1.10	1 (5%)
3	NAG	C	802	1	14,14,15	1.16	2 (14%)	17,19,21	0.68	0
3	NAG	C	804	1	14,14,15	1.11	1 (7%)	17,19,21	1.23	3 (17%)
3	NAG	C	803	1	14,14,15	1.30	2 (14%)	17,19,21	0.82	0
3	NAG	C	806	1	14,14,15	1.10	1 (7%)	17,19,21	0.62	0
3	NAG	A	802	1	14,14,15	1.17	2 (14%)	17,19,21	0.68	0
3	NAG	B	807	1	14,14,15	1.24	2 (14%)	17,19,21	0.78	0
3	NAG	A	808	1	14,14,15	1.22	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	A	805	1	14,14,15	1.21	1 (7%)	17,19,21	0.60	0
3	NAG	C	809	-	14,14,15	1.39	3 (21%)	17,19,21	1.09	1 (5%)
3	NAG	A	804	1	14,14,15	1.12	2 (14%)	17,19,21	1.24	3 (17%)
3	NAG	A	806	1	14,14,15	1.10	1 (7%)	17,19,21	0.62	0
3	NAG	B	804	1	14,14,15	1.12	2 (14%)	17,19,21	1.24	3 (17%)
3	NAG	B	808	1	14,14,15	1.22	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	B	805	1	14,14,15	1.21	1 (7%)	17,19,21	0.60	0
3	NAG	B	802	1	14,14,15	1.17	2 (14%)	17,19,21	0.69	0
3	NAG	B	806	1	14,14,15	1.10	1 (7%)	17,19,21	0.62	0
3	NAG	C	807	1	14,14,15	1.26	2 (14%)	17,19,21	0.78	0
3	NAG	A	803	1	14,14,15	1.30	2 (14%)	17,19,21	0.82	0
3	NAG	B	803	1	14,14,15	1.30	2 (14%)	17,19,21	0.82	0
3	NAG	A	807	1	14,14,15	1.25	2 (14%)	17,19,21	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	801	1	-	1/6/23/26	0/1/1/1
3	NAG	A	809	-	-	2/6/23/26	0/1/1/1
3	NAG	B	801	1	-	1/6/23/26	0/1/1/1
3	NAG	A	801	1	-	1/6/23/26	0/1/1/1
3	NAG	C	808	1	-	0/6/23/26	0/1/1/1
3	NAG	C	805	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	809	-	-	2/6/23/26	0/1/1/1
3	NAG	C	802	1	-	0/6/23/26	0/1/1/1
3	NAG	C	804	1	-	2/6/23/26	0/1/1/1
3	NAG	C	803	1	-	3/6/23/26	0/1/1/1
3	NAG	C	806	1	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	807	1	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
3	NAG	A	805	1	-	1/6/23/26	0/1/1/1
3	NAG	C	809	-	-	2/6/23/26	0/1/1/1
3	NAG	A	804	1	-	2/6/23/26	0/1/1/1
3	NAG	A	806	1	-	0/6/23/26	0/1/1/1
3	NAG	B	804	1	-	2/6/23/26	0/1/1/1
3	NAG	B	808	1	-	0/6/23/26	0/1/1/1
3	NAG	B	805	1	-	1/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	806	1	-	0/6/23/26	0/1/1/1
3	NAG	C	807	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	3/6/23/26	0/1/1/1
3	NAG	B	803	1	-	3/6/23/26	0/1/1/1
3	NAG	A	807	1	-	0/6/23/26	0/1/1/1

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	809	NAG	O5-C5	3.05	1.49	1.43
3	A	809	NAG	O5-C5	3.04	1.49	1.43
3	B	809	NAG	O5-C5	3.03	1.49	1.43
3	B	808	NAG	O5-C5	2.82	1.48	1.43
3	A	808	NAG	O5-C5	2.82	1.48	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	808	NAG	C1-O5-C5	2.94	116.13	112.19
3	A	808	NAG	C1-O5-C5	2.93	116.12	112.19
3	B	808	NAG	C1-O5-C5	2.92	116.10	112.19
3	B	804	NAG	C1-C2-N2	2.86	114.94	110.43
3	A	804	NAG	C1-C2-N2	2.86	114.94	110.43

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	NAG	O5-C5-C6-O6
3	B	803	NAG	O5-C5-C6-O6
3	C	803	NAG	O5-C5-C6-O6
3	A	801	NAG	O5-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	809	NAG	5	0
3	B	809	NAG	5	0
3	C	809	NAG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

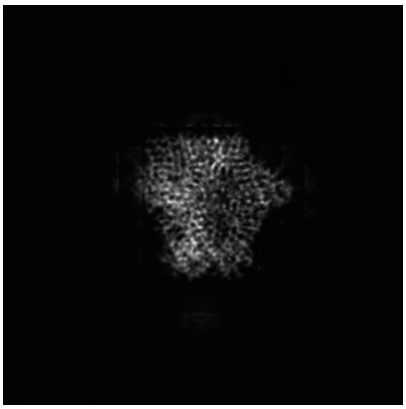
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28608. These allow visual inspection of the internal detail of the map and identification of artifacts.

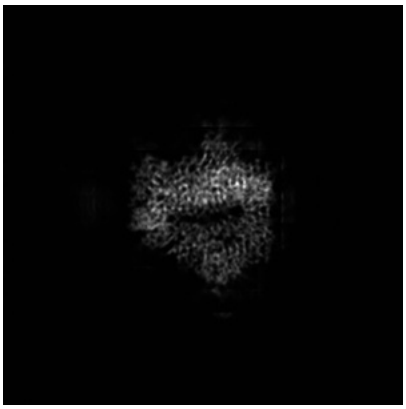
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

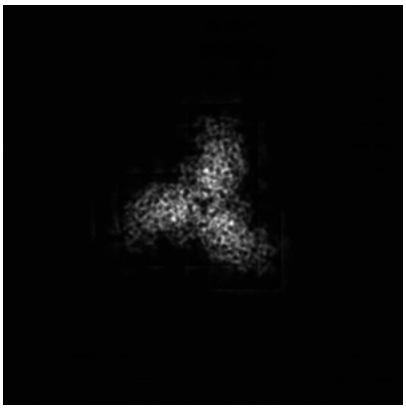
6.1.1 Primary map



X

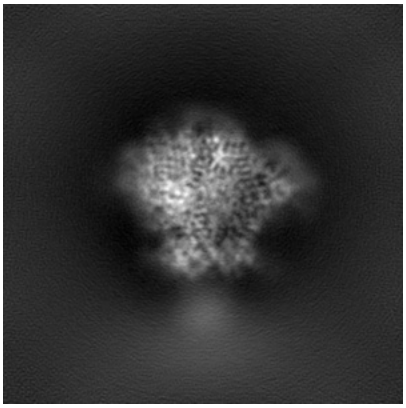


Y

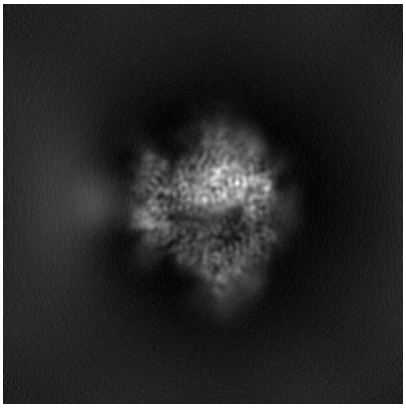


Z

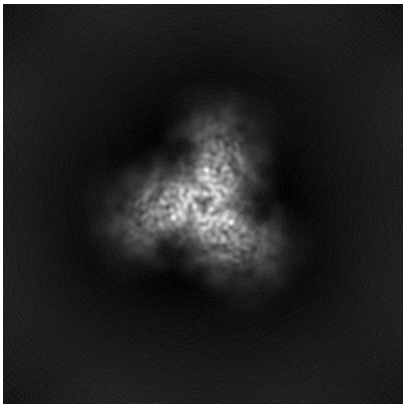
6.1.2 Raw map



X



Y

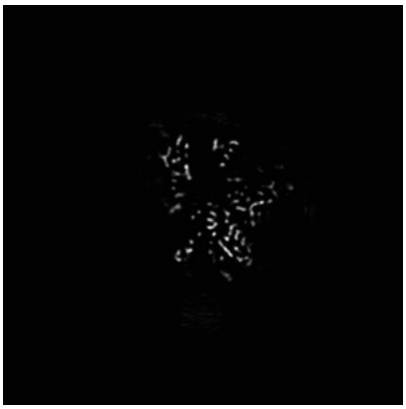


Z

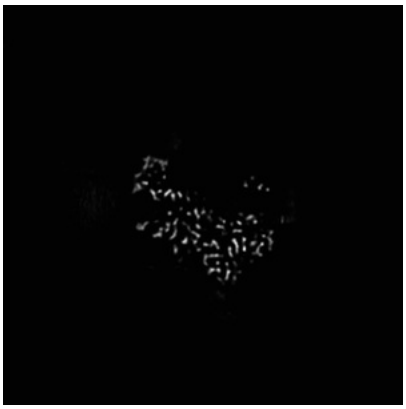
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



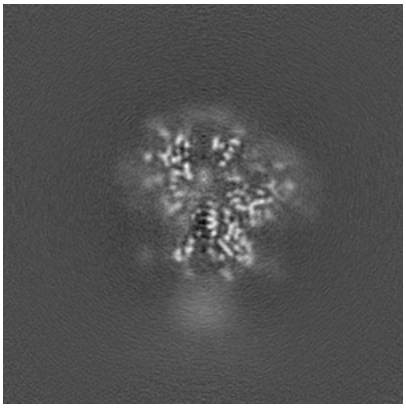
X Index: 128



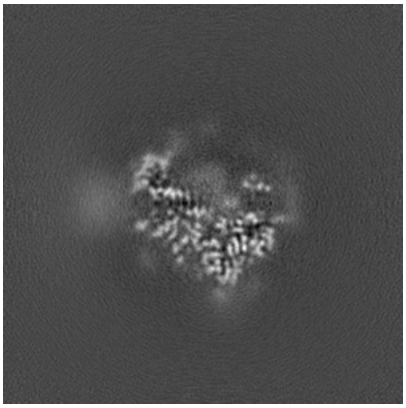
Y Index: 128

Z Index: 128

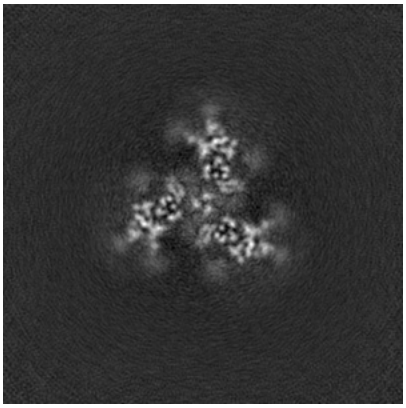
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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

6.3 Largest variance slices (i)

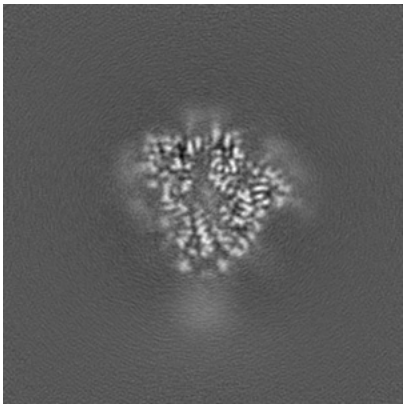
6.3.1 Primary map

X Index: 135

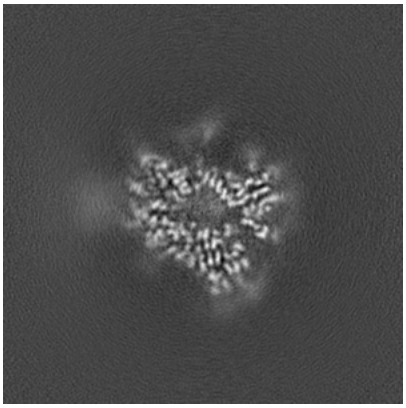
Y Index: 120

Z Index: 137

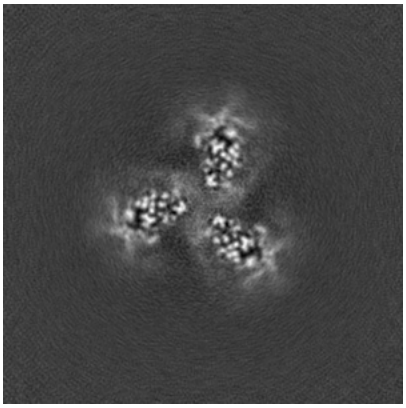
6.3.2 Raw map



X Index: 135



Y Index: 118

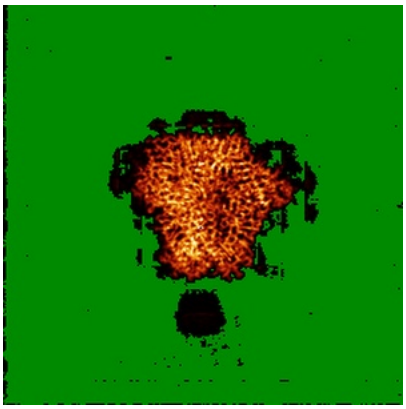


Z Index: 137

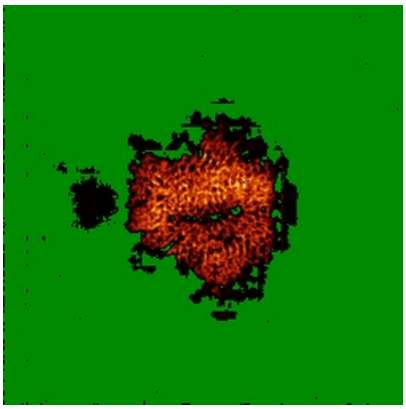
The images above show the largest variance slices of the map in three orthogonal directions.

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

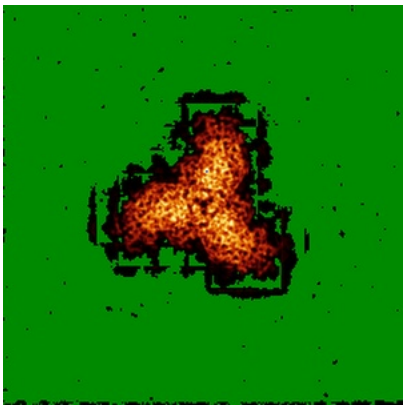
6.4.1 Primary map



X

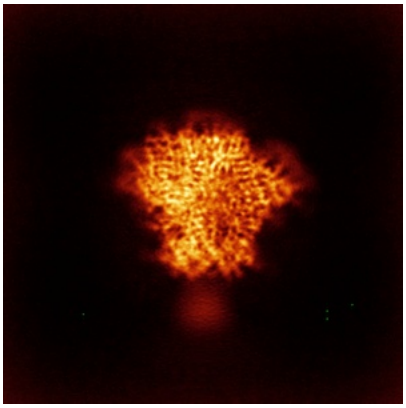


Y

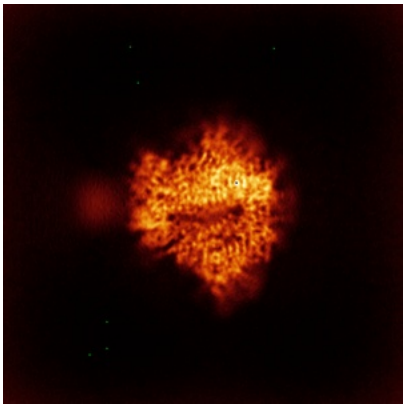


Z

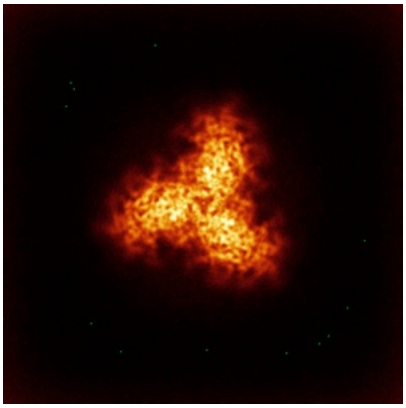
6.4.2 Raw map



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.

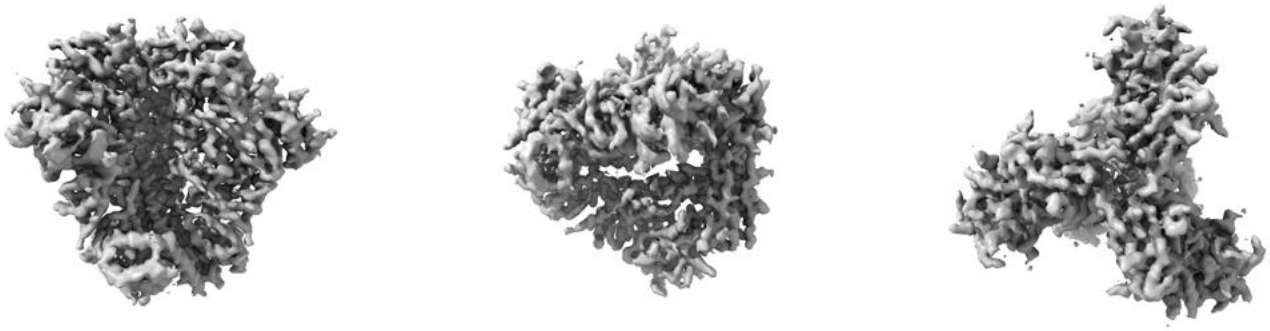
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

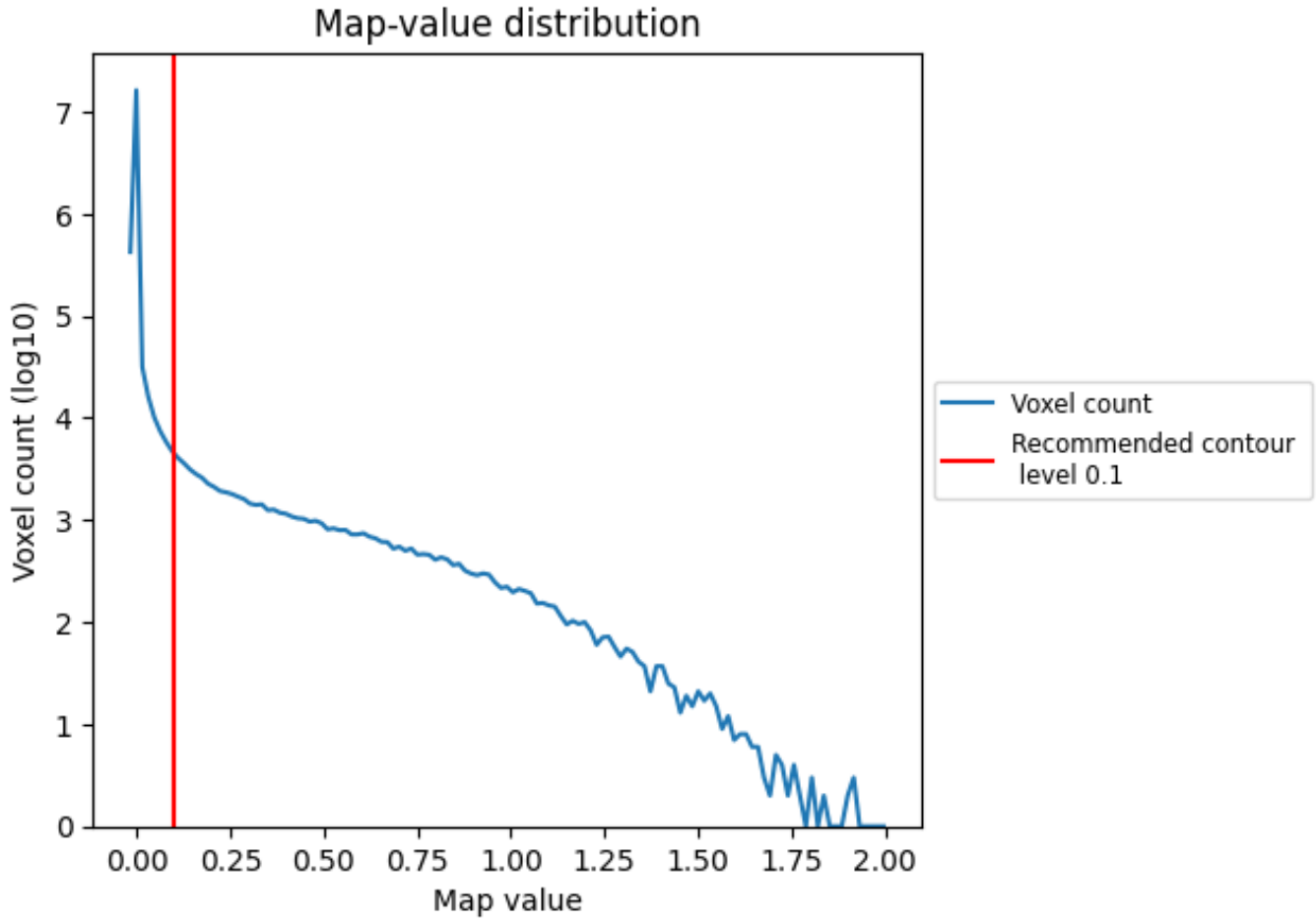
6.6 Mask visualisation (i)

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

7 Map analysis

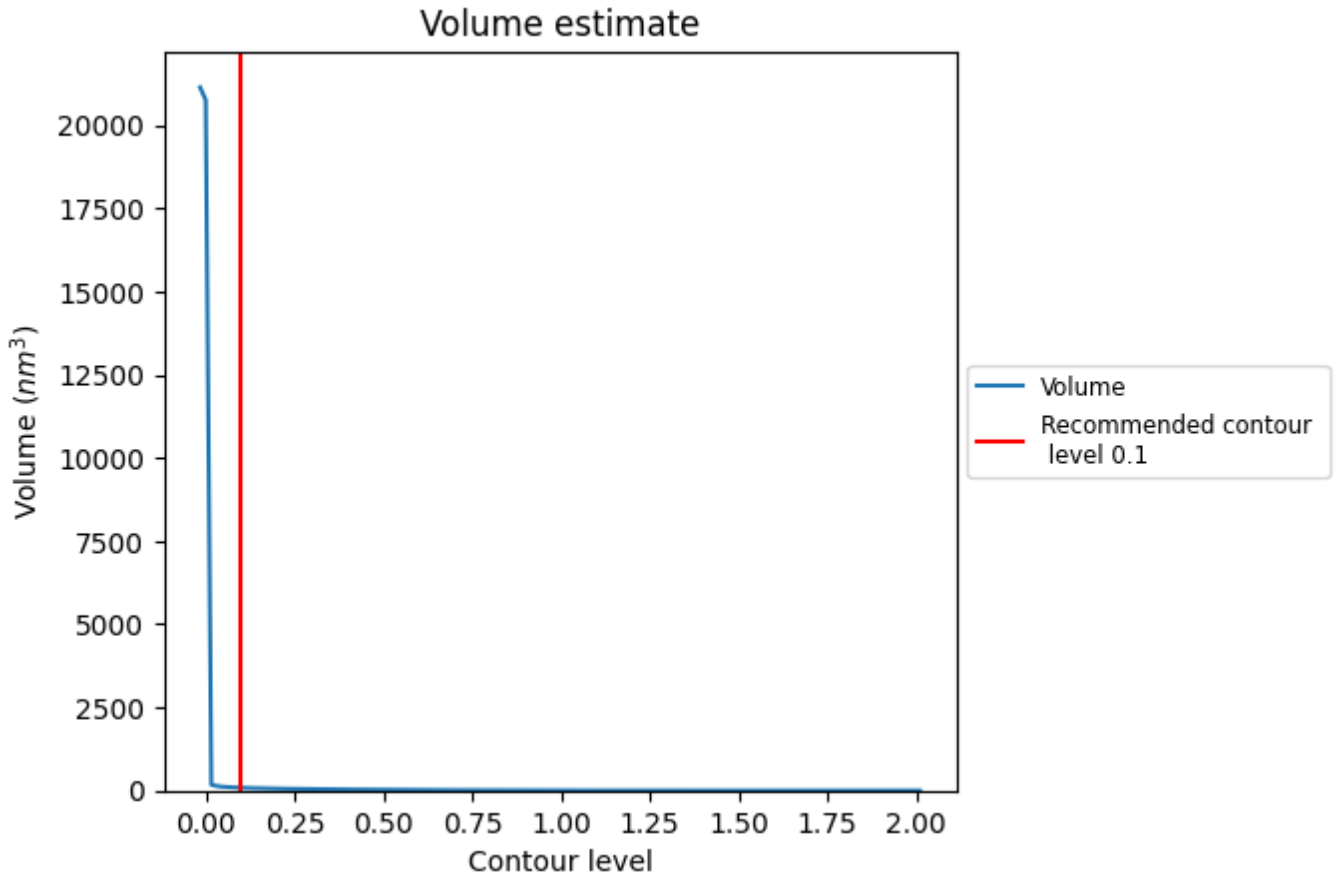
This section contains the results of statistical analysis of the map.

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.

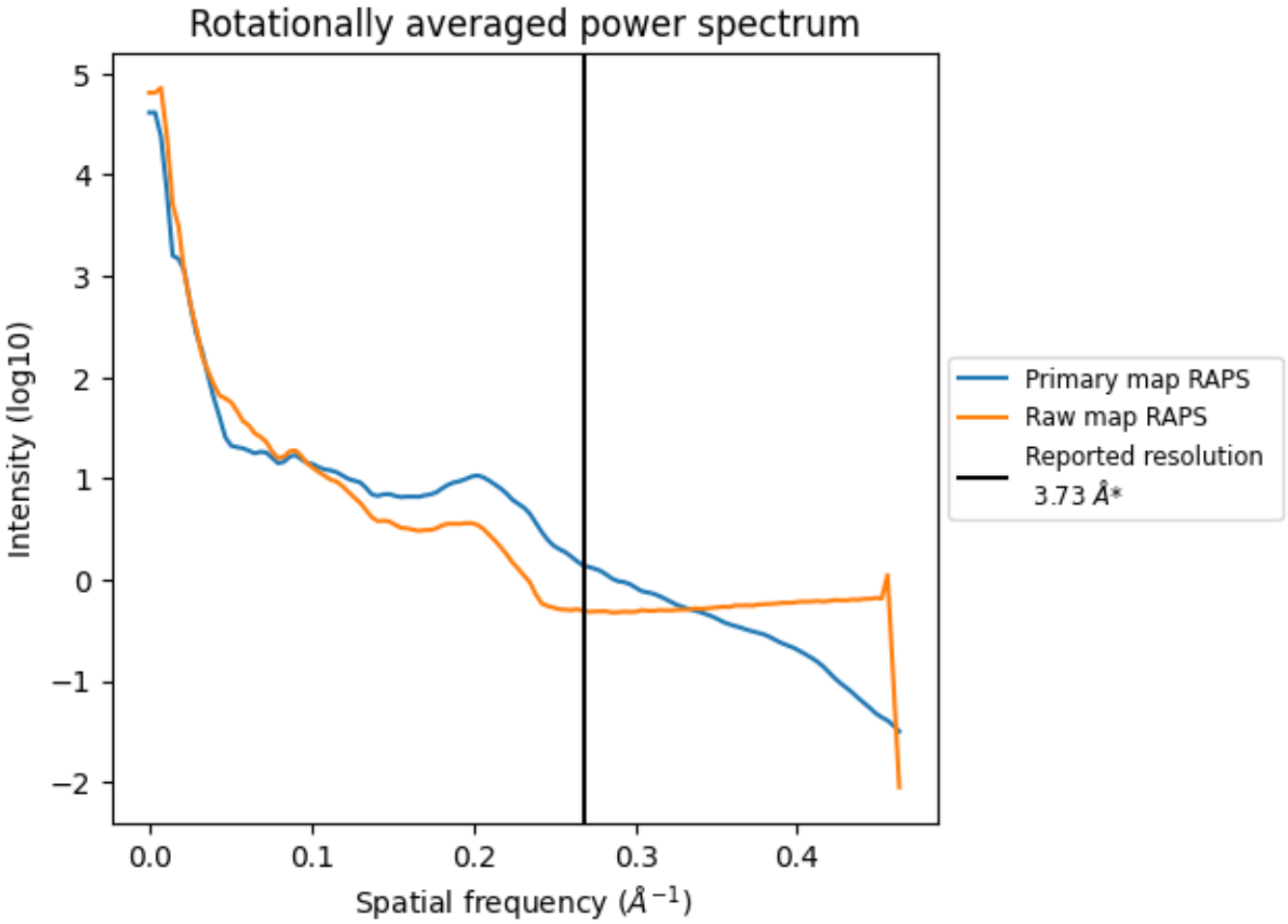
7.2 Volume estimate (i)



The volume at the recommended contour level is 84 nm^3; this corresponds to an approximate mass of 76 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)

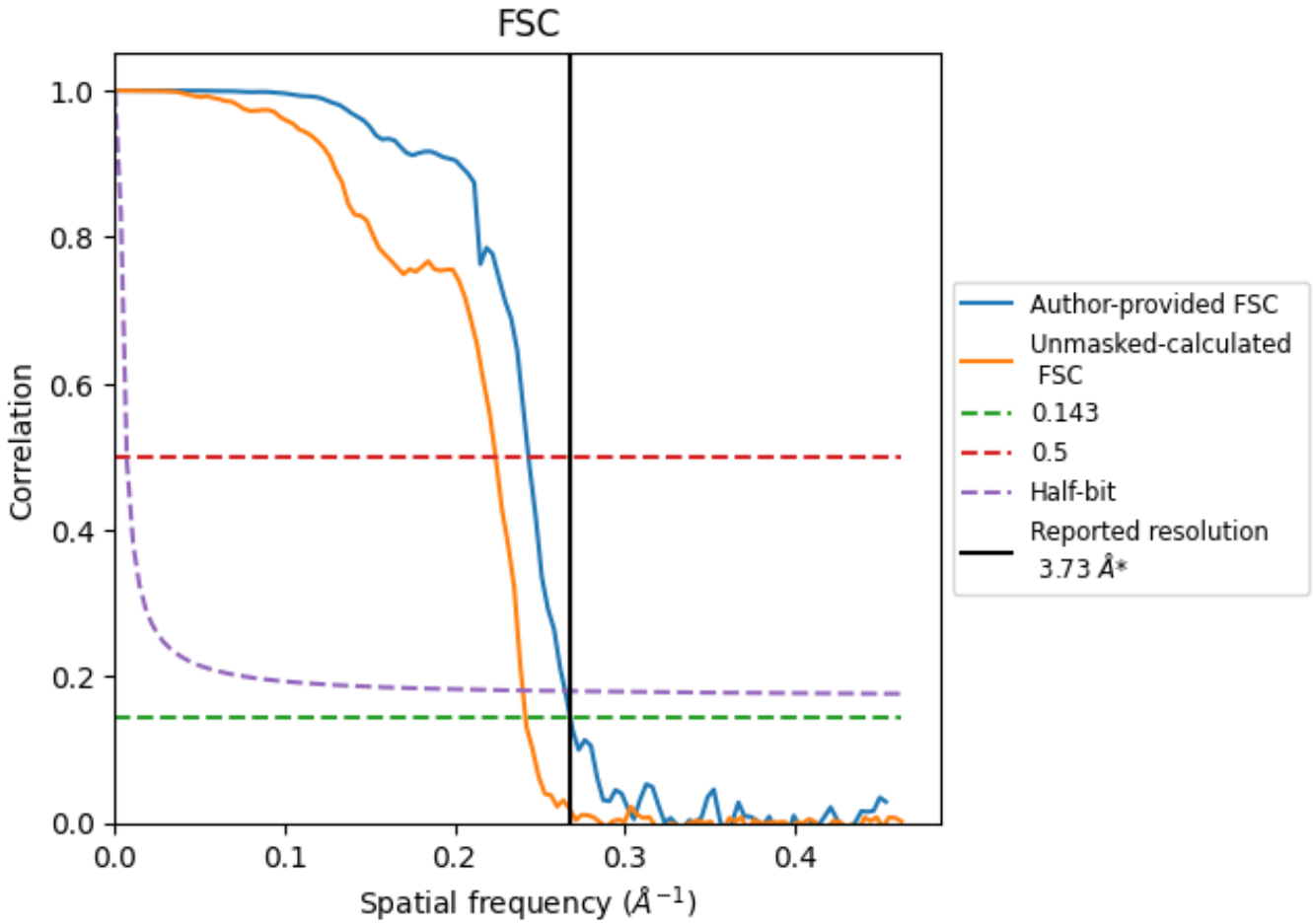


*Reported resolution corresponds to spatial frequency of 0.268 Å^{-1}

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 0.268 Å^{-1}

8.2 Resolution estimates (i)

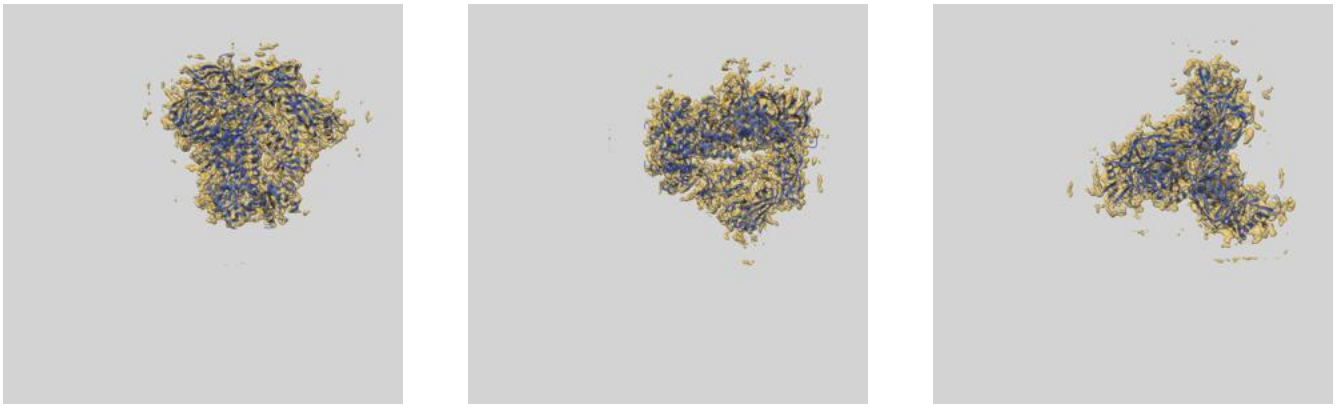
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	3.73	4.11	3.77
Unmasked-calculated*	4.14	4.46	4.16

*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 4.14 differs from the reported value 3.73 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28608 and PDB model 8EU8. Per-residue inclusion information can be found in section 3 on page 16.

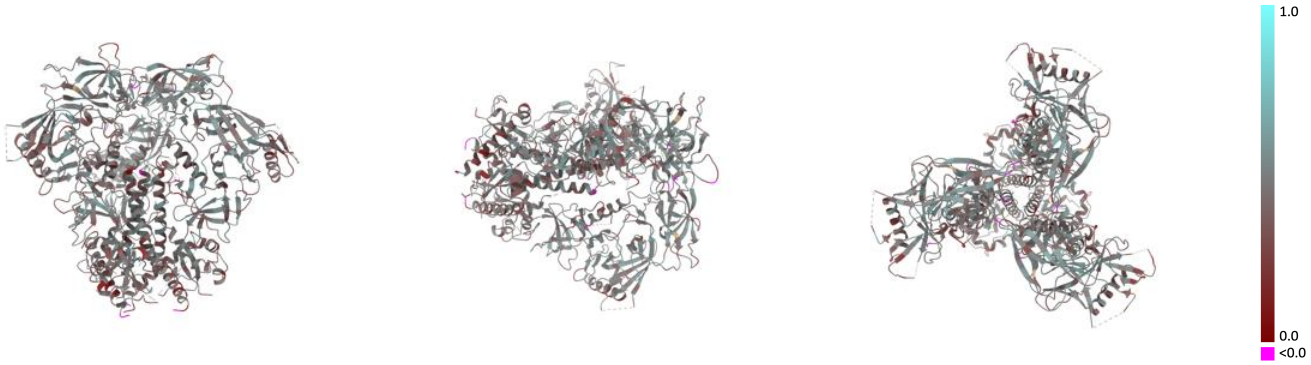
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

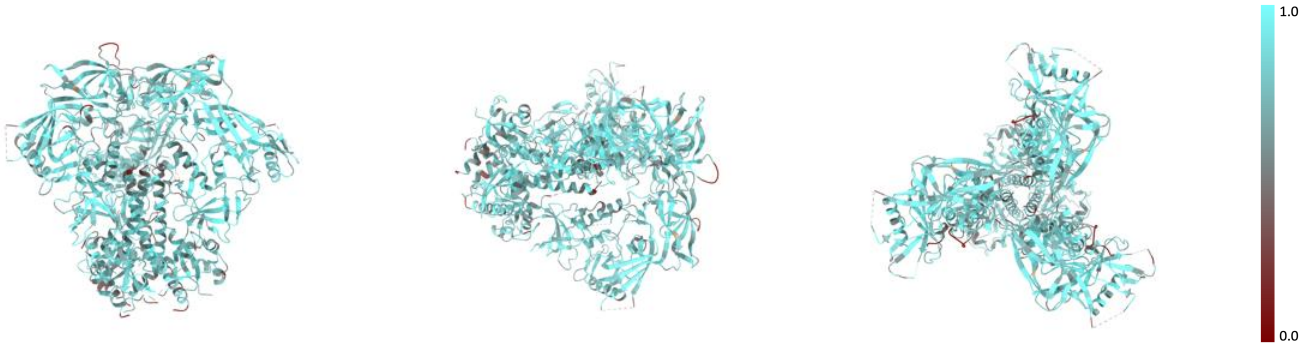
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

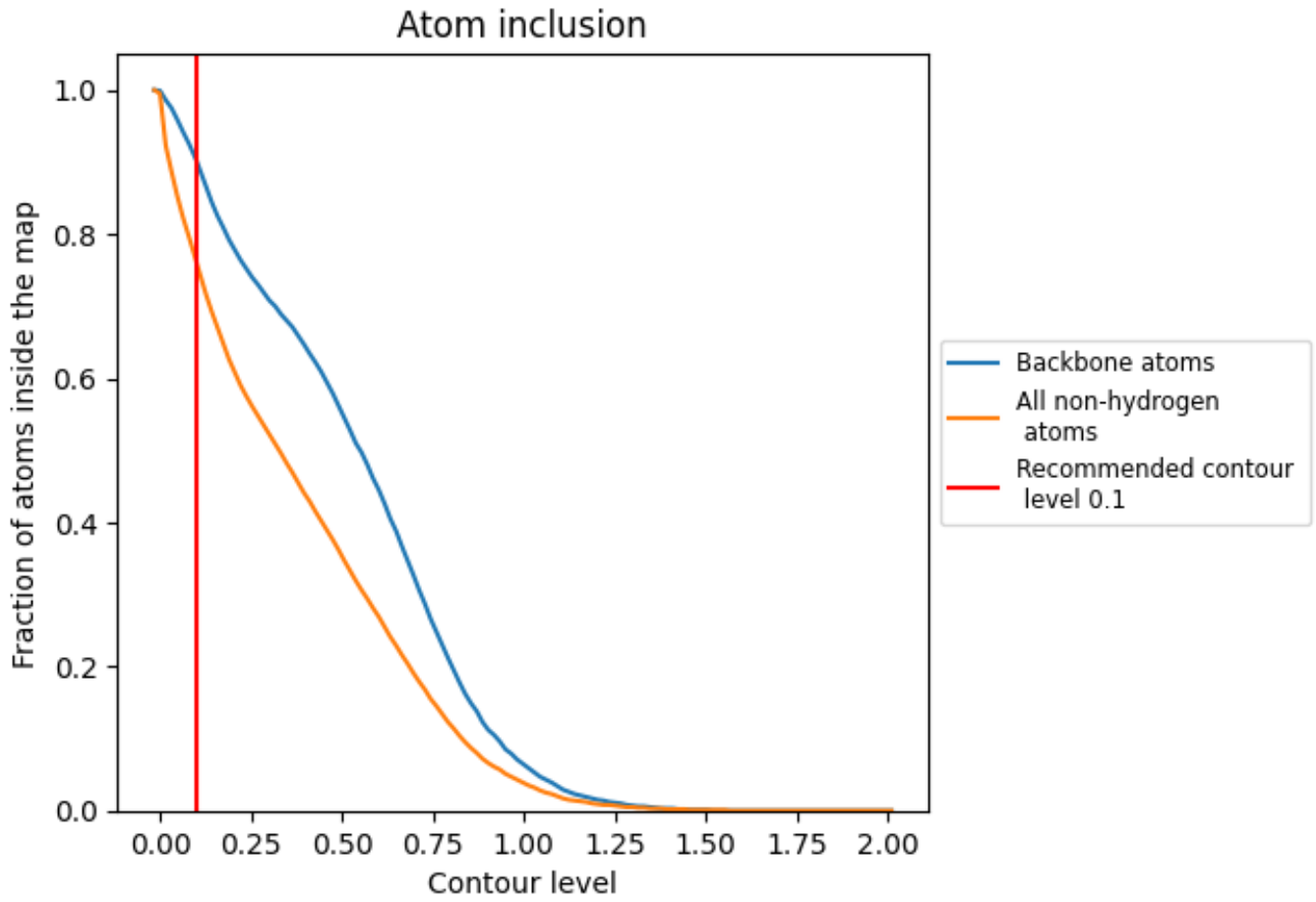
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.4310
A	0.7780	0.4370
B	0.7690	0.4320
C	0.7660	0.4330
D	0.6790	0.4690
E	0.4640	0.2680
F	0.7860	0.5020
G	0.2860	0.2620
H	0.3210	0.3610
I	0.3570	0.2090
J	0.4640	0.4310
K	0.3570	0.2820
L	0.7500	0.4790
M	0.3930	0.2950
N	0.5710	0.3920
O	0.2140	0.2610
P	0.6430	0.4720
Q	0.4290	0.2930
R	0.7140	0.4920
S	0.1790	0.2330
T	0.6430	0.3800
U	0.3210	0.2140