wwPDB EM Validation Summary Report

Sep 7, 2024 – 04:24 PM EDT

PDB ID	:	8VYM
EMDB ID	:	EMD-43667
Title	:	Soluble ectodomain of human cytomegalovirus (HCMV) glycoprotein B (gB) in the postfusion conformation in complex with 1G2 and 7H3 Fabs
Authors	:	Sponholtz, M.R.; Byrne, P.O.; McLellan, J.S.
Deposited on	:	2024-02-09
Resolution	:	3.40 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:

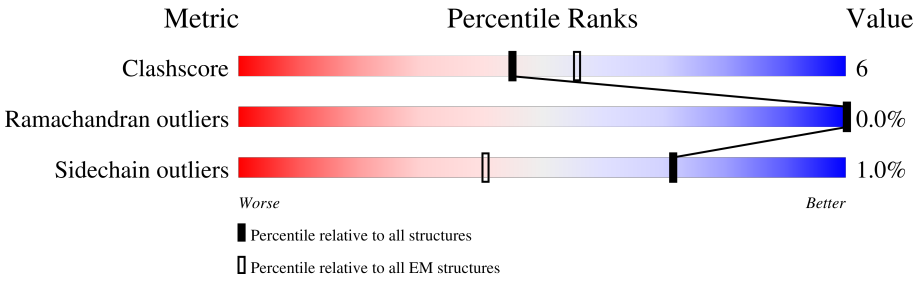
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	786	9% 49% 7% 44%
1	B	786	10% 45% 9% 46%
1	C	786	9% 48% 8% 44%
2	D	224	25% 45% 8% 47%
2	G	224	14% 37% 16% 47%
2	J	224	19% 40% 12% 47%
3	E	214	15% 43% 6% 50%
3	F	214	6% 44% 6% 50%

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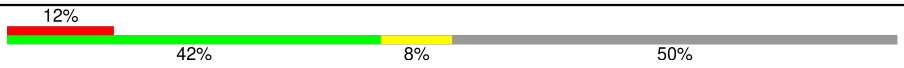
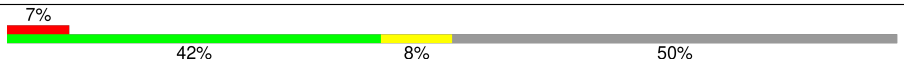
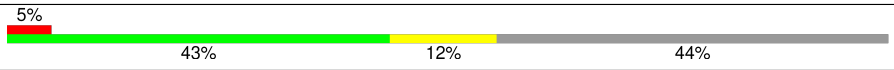
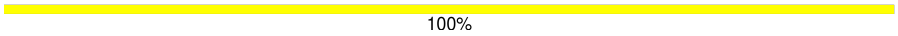
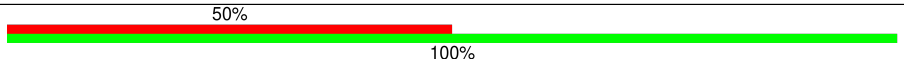
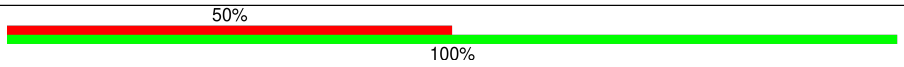
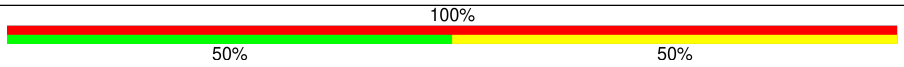
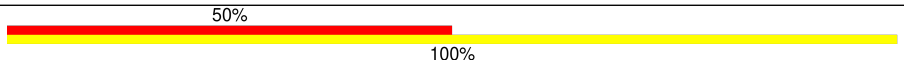
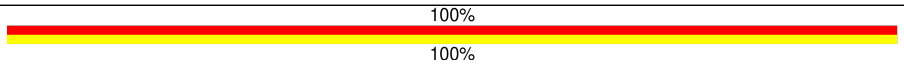
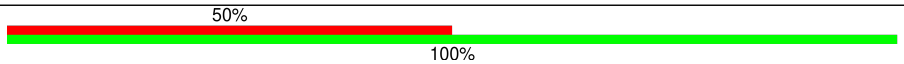
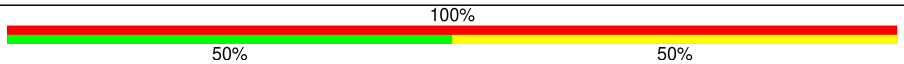
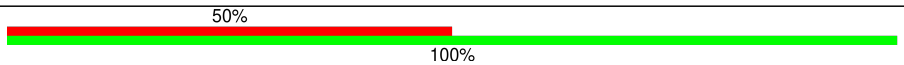
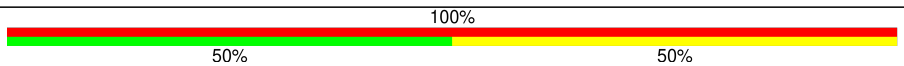
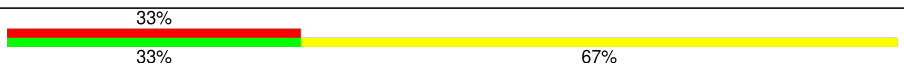
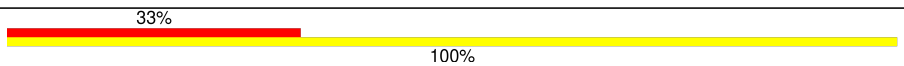
Mol	Chain	Length	Quality of chain
3	I	214	
4	H	216	
5	K	234	
6	L	2	
6	M	2	
6	N	2	
6	O	2	
6	P	2	
6	Q	2	
6	S	2	
6	T	2	
6	U	2	
6	X	2	
6	Y	2	
6	Z	2	
6	a	2	
7	R	3	
7	V	3	
7	W	3	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 18289 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	442	Total	C	N	O	S	0	0
			3591	2268	613	693	17		
1	B	425	Total	C	N	O	S	0	0
			3461	2194	583	667	17		
1	C	440	Total	C	N	O	S	0	0
			3574	2257	607	693	17		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	SER	CYS	conflict	UNP P13201
A	457	SER	ARG	conflict	UNP P13201
A	460	SER	ARG	conflict	UNP P13201
A	705	GLY	-	expression tag	UNP P13201
A	706	SER	-	expression tag	UNP P13201
A	707	GLY	-	expression tag	UNP P13201
A	708	TYR	-	expression tag	UNP P13201
A	709	ILE	-	expression tag	UNP P13201
A	710	PRO	-	expression tag	UNP P13201
A	711	GLU	-	expression tag	UNP P13201
A	712	ALA	-	expression tag	UNP P13201
A	713	PRO	-	expression tag	UNP P13201
A	714	ARG	-	expression tag	UNP P13201
A	715	ASP	-	expression tag	UNP P13201
A	716	GLY	-	expression tag	UNP P13201
A	717	GLN	-	expression tag	UNP P13201
A	718	ALA	-	expression tag	UNP P13201
A	719	TYR	-	expression tag	UNP P13201
A	720	VAL	-	expression tag	UNP P13201
A	721	ARG	-	expression tag	UNP P13201
A	722	LYS	-	expression tag	UNP P13201
A	723	ASP	-	expression tag	UNP P13201
A	724	GLY	-	expression tag	UNP P13201
A	725	GLU	-	expression tag	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
A	726	TRP	-	expression tag	UNP P13201
A	727	VAL	-	expression tag	UNP P13201
A	728	LEU	-	expression tag	UNP P13201
A	729	LEU	-	expression tag	UNP P13201
A	730	SER	-	expression tag	UNP P13201
A	731	THR	-	expression tag	UNP P13201
A	732	PHE	-	expression tag	UNP P13201
A	733	LEU	-	expression tag	UNP P13201
A	734	GLY	-	expression tag	UNP P13201
A	735	ALA	-	expression tag	UNP P13201
A	736	ALA	-	expression tag	UNP P13201
A	737	ALA	-	expression tag	UNP P13201
A	738	SER	-	expression tag	UNP P13201
A	739	LEU	-	expression tag	UNP P13201
A	740	GLU	-	expression tag	UNP P13201
A	741	VAL	-	expression tag	UNP P13201
A	742	LEU	-	expression tag	UNP P13201
A	743	PHE	-	expression tag	UNP P13201
A	744	GLN	-	expression tag	UNP P13201
A	745	GLY	-	expression tag	UNP P13201
A	746	PRO	-	expression tag	UNP P13201
A	747	GLY	-	expression tag	UNP P13201
A	748	HIS	-	expression tag	UNP P13201
A	749	HIS	-	expression tag	UNP P13201
A	750	HIS	-	expression tag	UNP P13201
A	751	HIS	-	expression tag	UNP P13201
A	752	HIS	-	expression tag	UNP P13201
A	753	HIS	-	expression tag	UNP P13201
A	754	HIS	-	expression tag	UNP P13201
A	755	HIS	-	expression tag	UNP P13201
A	756	SER	-	expression tag	UNP P13201
A	757	ALA	-	expression tag	UNP P13201
A	758	TRP	-	expression tag	UNP P13201
A	759	SER	-	expression tag	UNP P13201
A	760	HIS	-	expression tag	UNP P13201
A	761	PRO	-	expression tag	UNP P13201
A	762	GLN	-	expression tag	UNP P13201
A	763	PHE	-	expression tag	UNP P13201
A	764	GLU	-	expression tag	UNP P13201
A	765	LYS	-	expression tag	UNP P13201
A	766	GLY	-	expression tag	UNP P13201
A	767	GLY	-	expression tag	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
A	768	ALA	-	expression tag	UNP P13201
A	769	SER	-	expression tag	UNP P13201
A	770	GLY	-	expression tag	UNP P13201
A	771	GLY	-	expression tag	UNP P13201
A	772	GLY	-	expression tag	UNP P13201
A	773	GLY	-	expression tag	UNP P13201
A	774	SER	-	expression tag	UNP P13201
A	775	GLY	-	expression tag	UNP P13201
A	776	GLY	-	expression tag	UNP P13201
A	777	SER	-	expression tag	UNP P13201
A	778	ALA	-	expression tag	UNP P13201
A	779	TRP	-	expression tag	UNP P13201
A	780	SER	-	expression tag	UNP P13201
A	781	HIS	-	expression tag	UNP P13201
A	782	PRO	-	expression tag	UNP P13201
A	783	GLN	-	expression tag	UNP P13201
A	784	PHE	-	expression tag	UNP P13201
A	785	GLU	-	expression tag	UNP P13201
A	786	LYS	-	expression tag	UNP P13201
B	246	SER	CYS	conflict	UNP P13201
B	457	SER	ARG	conflict	UNP P13201
B	460	SER	ARG	conflict	UNP P13201
B	705	GLY	-	expression tag	UNP P13201
B	706	SER	-	expression tag	UNP P13201
B	707	GLY	-	expression tag	UNP P13201
B	708	TYR	-	expression tag	UNP P13201
B	709	ILE	-	expression tag	UNP P13201
B	710	PRO	-	expression tag	UNP P13201
B	711	GLU	-	expression tag	UNP P13201
B	712	ALA	-	expression tag	UNP P13201
B	713	PRO	-	expression tag	UNP P13201
B	714	ARG	-	expression tag	UNP P13201
B	715	ASP	-	expression tag	UNP P13201
B	716	GLY	-	expression tag	UNP P13201
B	717	GLN	-	expression tag	UNP P13201
B	718	ALA	-	expression tag	UNP P13201
B	719	TYR	-	expression tag	UNP P13201
B	720	VAL	-	expression tag	UNP P13201
B	721	ARG	-	expression tag	UNP P13201
B	722	LYS	-	expression tag	UNP P13201
B	723	ASP	-	expression tag	UNP P13201
B	724	GLY	-	expression tag	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
B	725	GLU	-	expression tag	UNP P13201
B	726	TRP	-	expression tag	UNP P13201
B	727	VAL	-	expression tag	UNP P13201
B	728	LEU	-	expression tag	UNP P13201
B	729	LEU	-	expression tag	UNP P13201
B	730	SER	-	expression tag	UNP P13201
B	731	THR	-	expression tag	UNP P13201
B	732	PHE	-	expression tag	UNP P13201
B	733	LEU	-	expression tag	UNP P13201
B	734	GLY	-	expression tag	UNP P13201
B	735	ALA	-	expression tag	UNP P13201
B	736	ALA	-	expression tag	UNP P13201
B	737	ALA	-	expression tag	UNP P13201
B	738	SER	-	expression tag	UNP P13201
B	739	LEU	-	expression tag	UNP P13201
B	740	GLU	-	expression tag	UNP P13201
B	741	VAL	-	expression tag	UNP P13201
B	742	LEU	-	expression tag	UNP P13201
B	743	PHE	-	expression tag	UNP P13201
B	744	GLN	-	expression tag	UNP P13201
B	745	GLY	-	expression tag	UNP P13201
B	746	PRO	-	expression tag	UNP P13201
B	747	GLY	-	expression tag	UNP P13201
B	748	HIS	-	expression tag	UNP P13201
B	749	HIS	-	expression tag	UNP P13201
B	750	HIS	-	expression tag	UNP P13201
B	751	HIS	-	expression tag	UNP P13201
B	752	HIS	-	expression tag	UNP P13201
B	753	HIS	-	expression tag	UNP P13201
B	754	HIS	-	expression tag	UNP P13201
B	755	HIS	-	expression tag	UNP P13201
B	756	SER	-	expression tag	UNP P13201
B	757	ALA	-	expression tag	UNP P13201
B	758	TRP	-	expression tag	UNP P13201
B	759	SER	-	expression tag	UNP P13201
B	760	HIS	-	expression tag	UNP P13201
B	761	PRO	-	expression tag	UNP P13201
B	762	GLN	-	expression tag	UNP P13201
B	763	PHE	-	expression tag	UNP P13201
B	764	GLU	-	expression tag	UNP P13201
B	765	LYS	-	expression tag	UNP P13201
B	766	GLY	-	expression tag	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
B	767	GLY	-	expression tag	UNP P13201
B	768	ALA	-	expression tag	UNP P13201
B	769	SER	-	expression tag	UNP P13201
B	770	GLY	-	expression tag	UNP P13201
B	771	GLY	-	expression tag	UNP P13201
B	772	GLY	-	expression tag	UNP P13201
B	773	GLY	-	expression tag	UNP P13201
B	774	SER	-	expression tag	UNP P13201
B	775	GLY	-	expression tag	UNP P13201
B	776	GLY	-	expression tag	UNP P13201
B	777	SER	-	expression tag	UNP P13201
B	778	ALA	-	expression tag	UNP P13201
B	779	TRP	-	expression tag	UNP P13201
B	780	SER	-	expression tag	UNP P13201
B	781	HIS	-	expression tag	UNP P13201
B	782	PRO	-	expression tag	UNP P13201
B	783	GLN	-	expression tag	UNP P13201
B	784	PHE	-	expression tag	UNP P13201
B	785	GLU	-	expression tag	UNP P13201
B	786	LYS	-	expression tag	UNP P13201
C	246	SER	CYS	conflict	UNP P13201
C	457	SER	ARG	conflict	UNP P13201
C	460	SER	ARG	conflict	UNP P13201
C	705	GLY	-	expression tag	UNP P13201
C	706	SER	-	expression tag	UNP P13201
C	707	GLY	-	expression tag	UNP P13201
C	708	TYR	-	expression tag	UNP P13201
C	709	ILE	-	expression tag	UNP P13201
C	710	PRO	-	expression tag	UNP P13201
C	711	GLU	-	expression tag	UNP P13201
C	712	ALA	-	expression tag	UNP P13201
C	713	PRO	-	expression tag	UNP P13201
C	714	ARG	-	expression tag	UNP P13201
C	715	ASP	-	expression tag	UNP P13201
C	716	GLY	-	expression tag	UNP P13201
C	717	GLN	-	expression tag	UNP P13201
C	718	ALA	-	expression tag	UNP P13201
C	719	TYR	-	expression tag	UNP P13201
C	720	VAL	-	expression tag	UNP P13201
C	721	ARG	-	expression tag	UNP P13201
C	722	LYS	-	expression tag	UNP P13201
C	723	ASP	-	expression tag	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
C	724	GLY	-	expression tag	UNP P13201
C	725	GLU	-	expression tag	UNP P13201
C	726	TRP	-	expression tag	UNP P13201
C	727	VAL	-	expression tag	UNP P13201
C	728	LEU	-	expression tag	UNP P13201
C	729	LEU	-	expression tag	UNP P13201
C	730	SER	-	expression tag	UNP P13201
C	731	THR	-	expression tag	UNP P13201
C	732	PHE	-	expression tag	UNP P13201
C	733	LEU	-	expression tag	UNP P13201
C	734	GLY	-	expression tag	UNP P13201
C	735	ALA	-	expression tag	UNP P13201
C	736	ALA	-	expression tag	UNP P13201
C	737	ALA	-	expression tag	UNP P13201
C	738	SER	-	expression tag	UNP P13201
C	739	LEU	-	expression tag	UNP P13201
C	740	GLU	-	expression tag	UNP P13201
C	741	VAL	-	expression tag	UNP P13201
C	742	LEU	-	expression tag	UNP P13201
C	743	PHE	-	expression tag	UNP P13201
C	744	GLN	-	expression tag	UNP P13201
C	745	GLY	-	expression tag	UNP P13201
C	746	PRO	-	expression tag	UNP P13201
C	747	GLY	-	expression tag	UNP P13201
C	748	HIS	-	expression tag	UNP P13201
C	749	HIS	-	expression tag	UNP P13201
C	750	HIS	-	expression tag	UNP P13201
C	751	HIS	-	expression tag	UNP P13201
C	752	HIS	-	expression tag	UNP P13201
C	753	HIS	-	expression tag	UNP P13201
C	754	HIS	-	expression tag	UNP P13201
C	755	HIS	-	expression tag	UNP P13201
C	756	SER	-	expression tag	UNP P13201
C	757	ALA	-	expression tag	UNP P13201
C	758	TRP	-	expression tag	UNP P13201
C	759	SER	-	expression tag	UNP P13201
C	760	HIS	-	expression tag	UNP P13201
C	761	PRO	-	expression tag	UNP P13201
C	762	GLN	-	expression tag	UNP P13201
C	763	PHE	-	expression tag	UNP P13201
C	764	GLU	-	expression tag	UNP P13201
C	765	LYS	-	expression tag	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
C	766	GLY	-	expression tag	UNP P13201
C	767	GLY	-	expression tag	UNP P13201
C	768	ALA	-	expression tag	UNP P13201
C	769	SER	-	expression tag	UNP P13201
C	770	GLY	-	expression tag	UNP P13201
C	771	GLY	-	expression tag	UNP P13201
C	772	GLY	-	expression tag	UNP P13201
C	773	GLY	-	expression tag	UNP P13201
C	774	SER	-	expression tag	UNP P13201
C	775	GLY	-	expression tag	UNP P13201
C	776	GLY	-	expression tag	UNP P13201
C	777	SER	-	expression tag	UNP P13201
C	778	ALA	-	expression tag	UNP P13201
C	779	TRP	-	expression tag	UNP P13201
C	780	SER	-	expression tag	UNP P13201
C	781	HIS	-	expression tag	UNP P13201
C	782	PRO	-	expression tag	UNP P13201
C	783	GLN	-	expression tag	UNP P13201
C	784	PHE	-	expression tag	UNP P13201
C	785	GLU	-	expression tag	UNP P13201
C	786	LYS	-	expression tag	UNP P13201

- Molecule 2 is a protein called 1G2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	118	Total	C	N	O	S	0	0
			944	608	158	176	2		
2	G	118	Total	C	N	O	S	0	0
			944	608	158	176	2		
2	J	118	Total	C	N	O	S	0	0
			944	608	158	176	2		

- Molecule 3 is a protein called 1G2 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	106	Total	C	N	O	S	0	0
			797	494	137	164	2		
3	F	106	Total	C	N	O	S	0	0
			797	494	137	164	2		
3	I	106	Total	C	N	O	S	0	0
			797	494	137	164	2		

- Molecule 4 is a protein called 7H3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	109	Total	C	N	O	S	0	0
			802	498	140	161	3		

- Molecule 5 is a protein called 7H3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	130	Total	C	N	O	S	0	0
			1017	643	170	197	7		

- Molecule 6 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
6	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	M	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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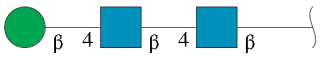
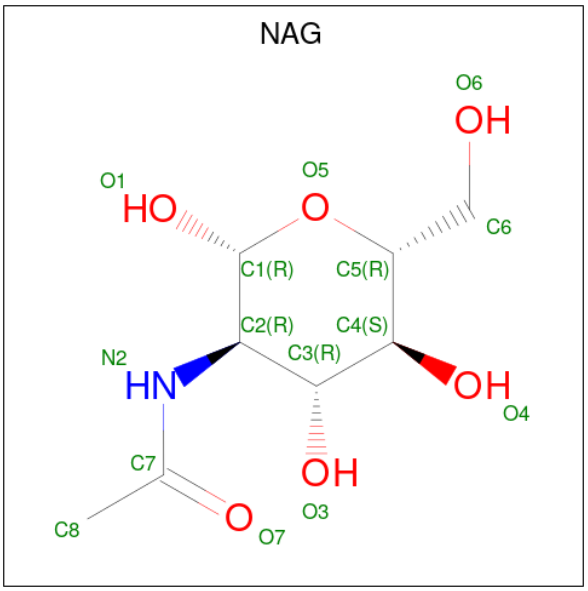
Mol	Chain	Residues	Atoms				AltConf	Trace
6	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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
7	R	3	Total	C	N	O	0	0
			39	22	2	15		
7	V	3	Total	C	N	O	0	0
			39	22	2	15		
7	W	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

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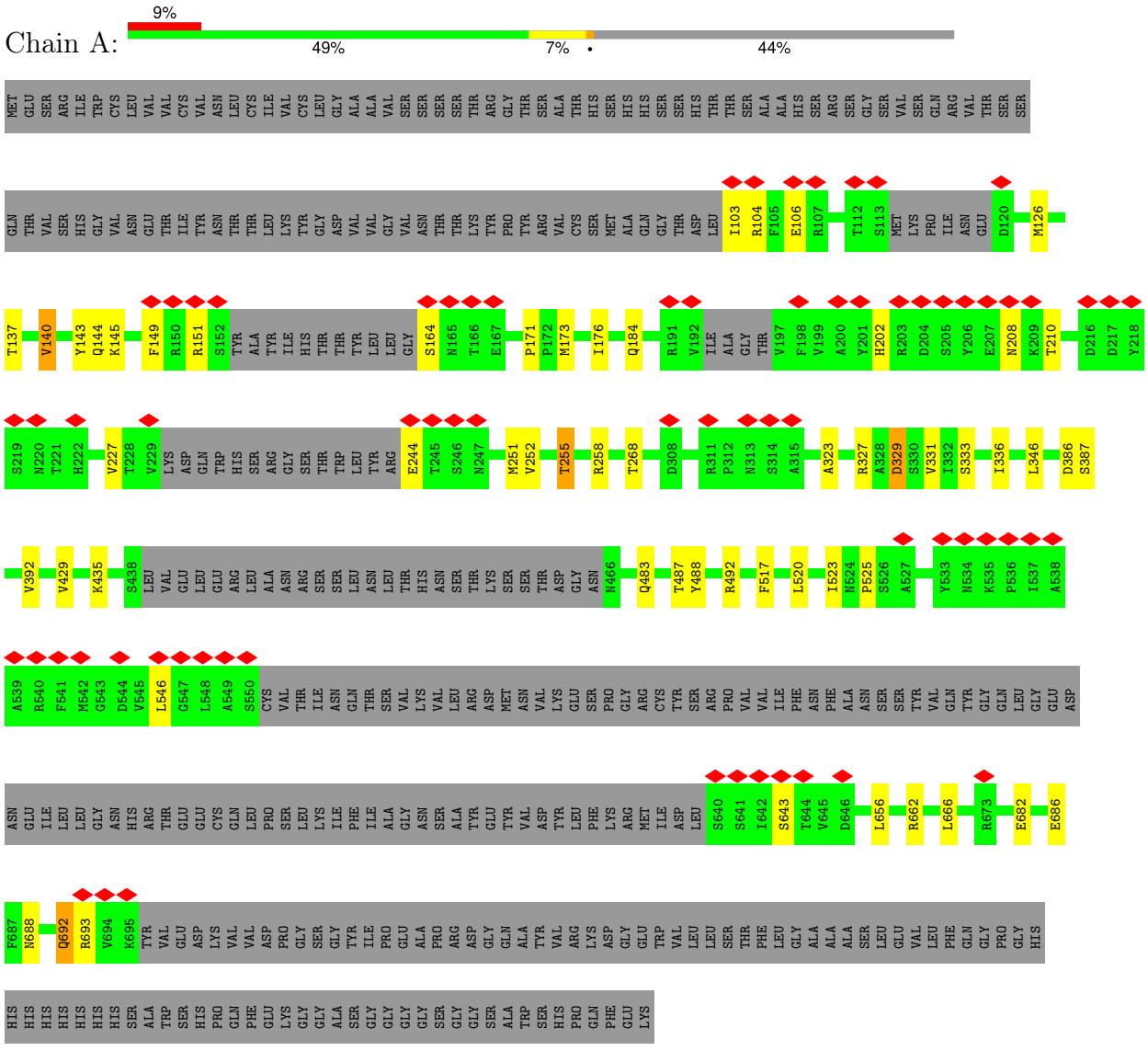
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	

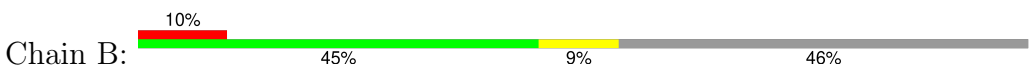
3 Residue-property plots (i)

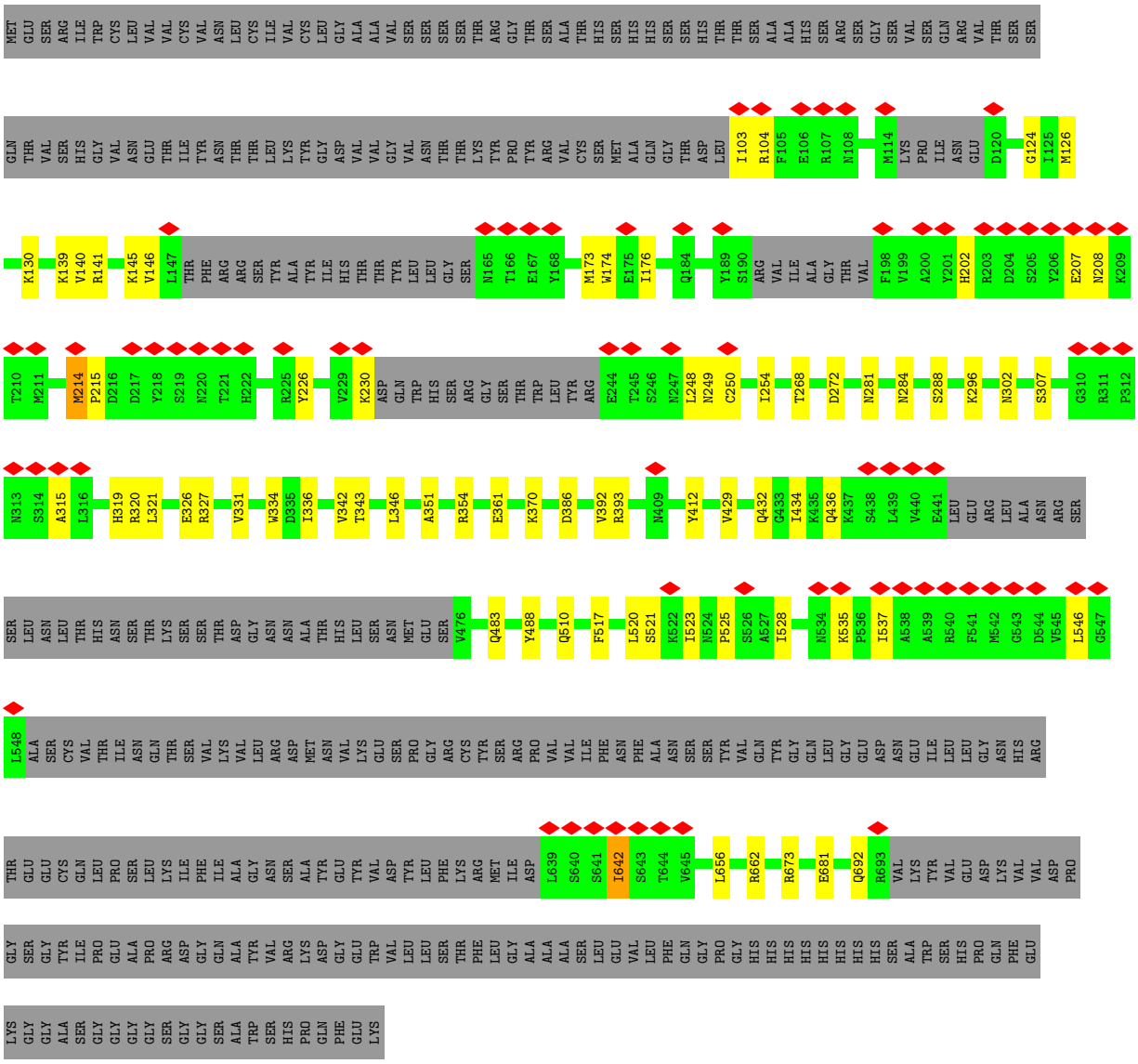
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Envelope glycoprotein B



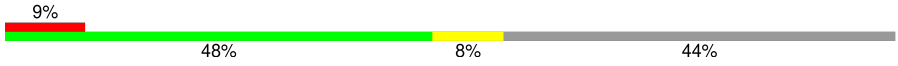
• Molecule 1: Envelope glycoprotein B

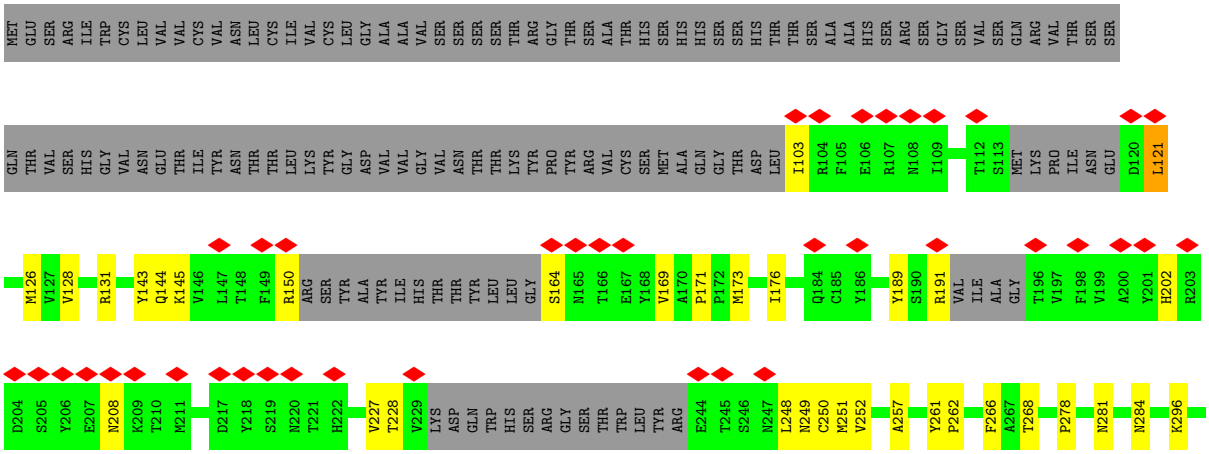


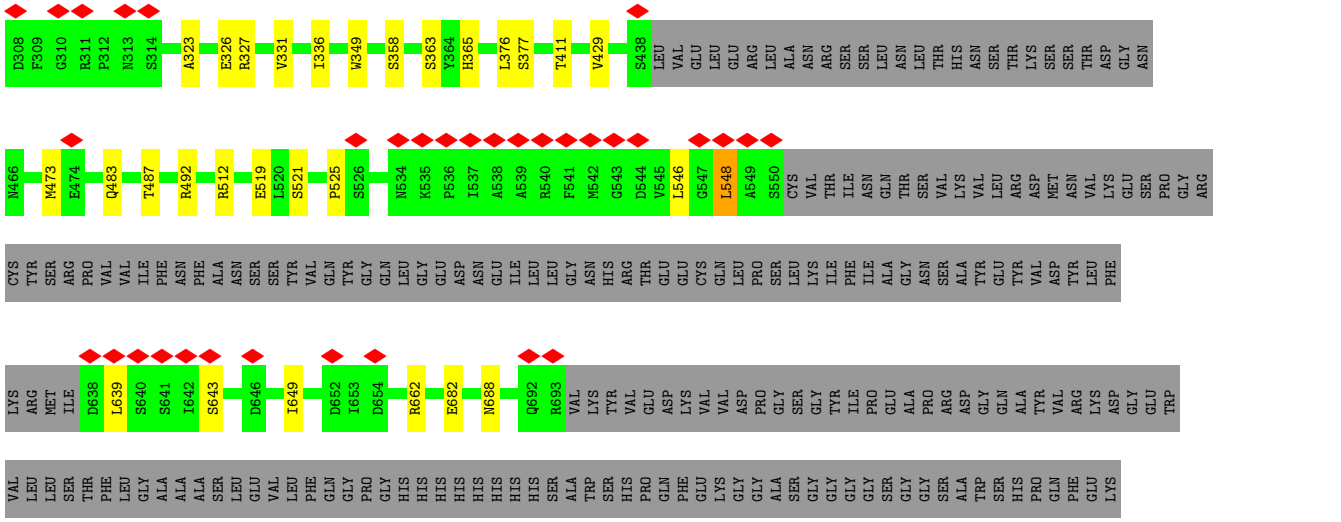


• Molecule 1: Envelope glycoprotein B

Chain C:

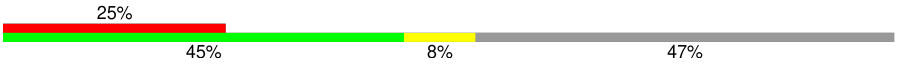


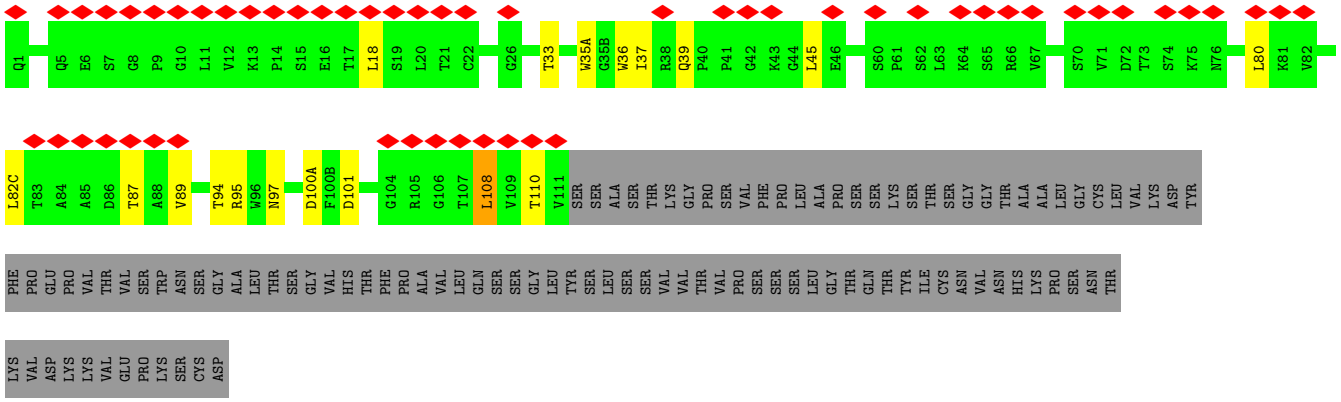




• Molecule 2: 1G2 Fab Heavy Chain

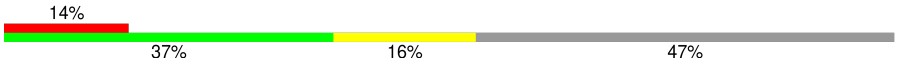
Chain D:

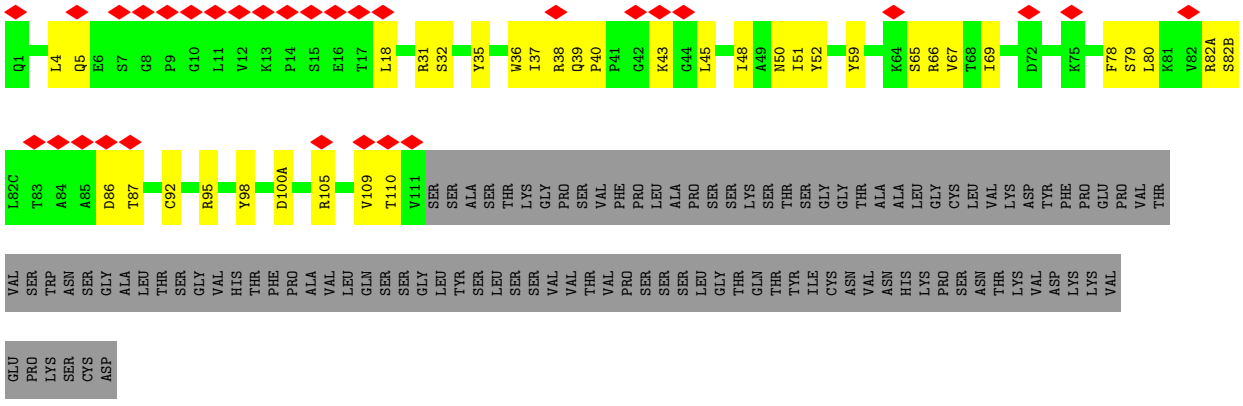




• Molecule 2: 1G2 Fab Heavy Chain

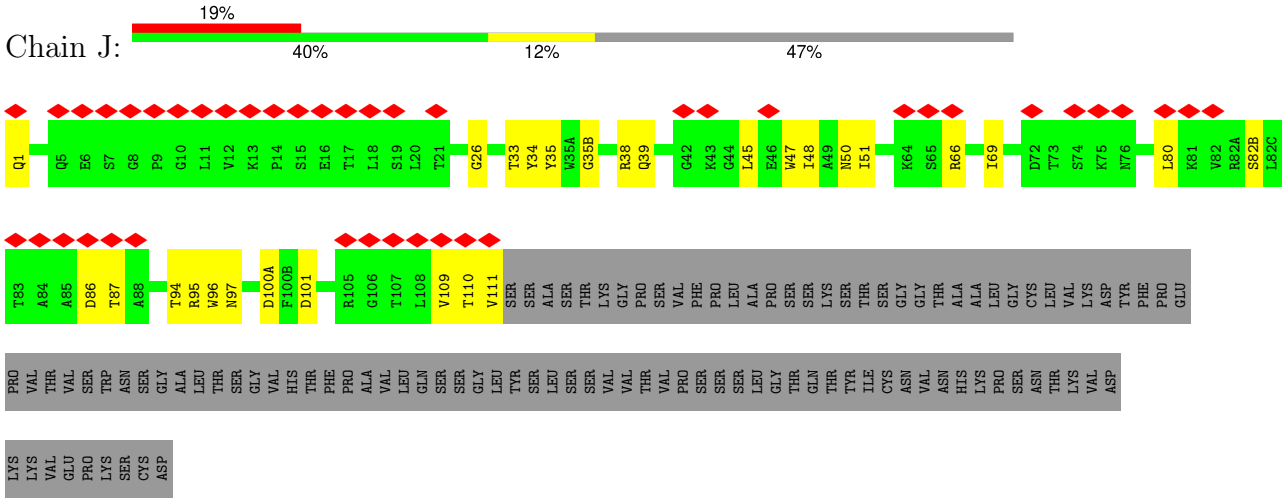
Chain G:





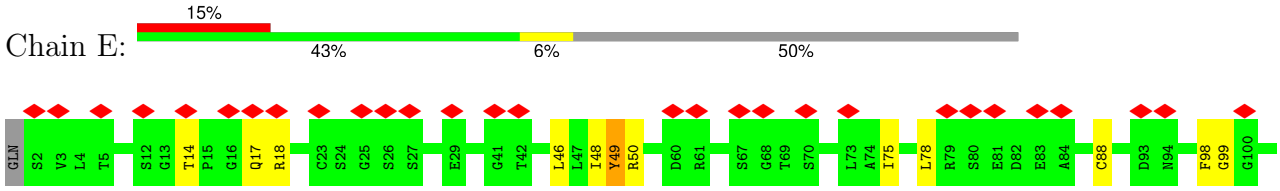
• Molecule 2: 1G2 Fab Heavy Chain

Chain J:



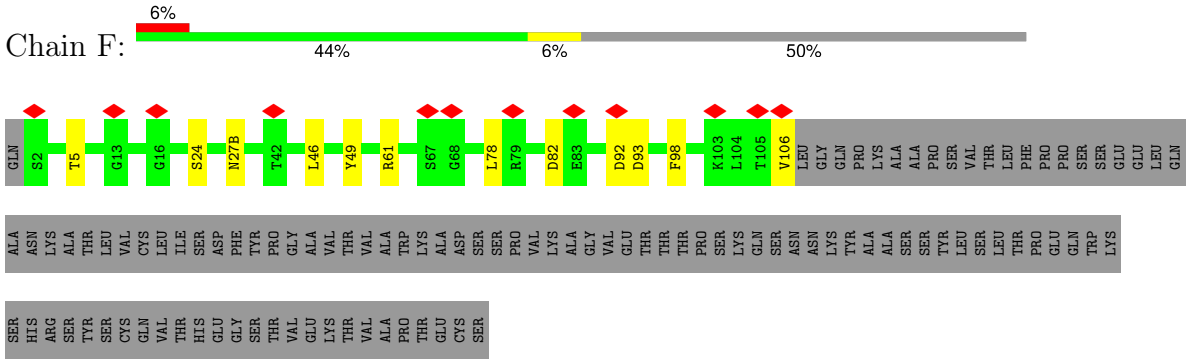
• Molecule 3: 1G2 Fab Light Chain

Chain E:



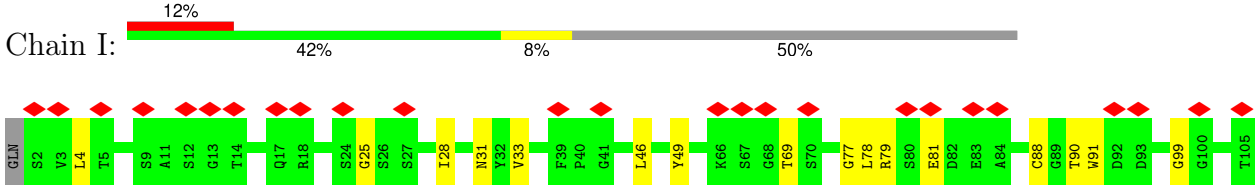
• Molecule 3: 1G2 Fab Light Chain

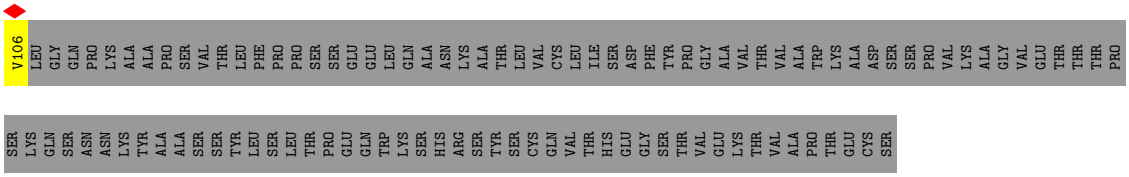
Chain F:



• Molecule 3: 1G2 Fab Light Chain

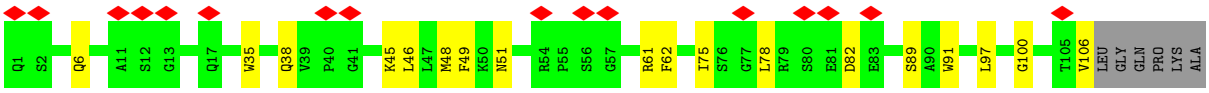
Chain I:





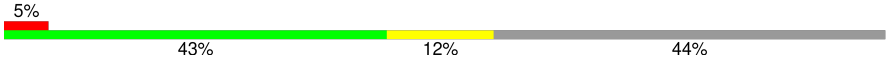
• Molecule 4: 7H3 Fab Light Chain

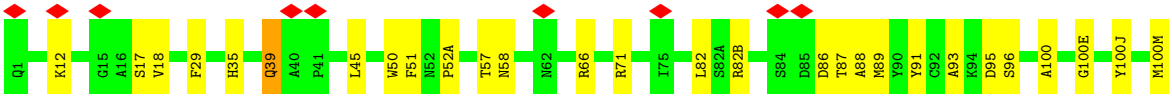
Chain H:



• Molecule 5: 7H3 Fab Heavy Chain

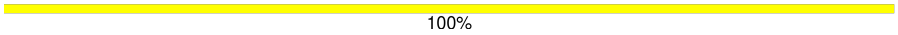
Chain K:





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

Chain L:



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

Chain M:

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

Chain N:

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

Chain O:

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

Chain P:

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

Chain Q:

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

Chain S:

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

Chain T:

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

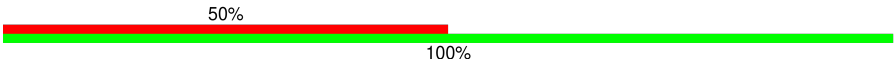
Chain U:

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

Chain X:

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

Chain Y:

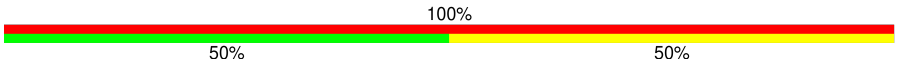


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

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

Chain a:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

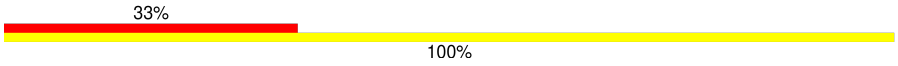
Chain R:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	211132	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.001	Depositor
Minimum map value	-0.641	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	426.59836, 426.59836, 426.59836	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8331999, 0.8331999, 0.8331999	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/3664	0.46	0/4956
1	B	0.25	0/3532	0.47	0/4778
1	C	0.25	0/3647	0.46	0/4935
2	D	0.25	0/971	0.49	0/1325
2	G	0.25	0/971	0.50	0/1325
2	J	0.25	0/971	0.50	0/1325
3	E	0.25	0/817	0.48	0/1113
3	F	0.25	0/817	0.48	0/1113
3	I	0.25	0/817	0.48	0/1113
4	H	0.26	0/821	0.49	0/1114
5	K	0.25	0/1044	0.48	0/1417
All	All	0.25	0/18072	0.47	0/24514

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3591	0	3451	42	0
1	B	3461	0	3328	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3574	0	3425	45	0
2	D	944	0	920	9	0
2	G	944	0	920	24	0
2	J	944	0	920	17	0
3	E	797	0	750	8	0
3	F	797	0	750	7	0
3	I	797	0	750	11	0
4	H	802	0	775	12	0
5	K	1017	0	953	19	0
6	L	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
6	O	28	0	25	0	0
6	P	28	0	25	0	0
6	Q	28	0	25	1	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	0	0
6	X	28	0	25	1	0
6	Y	28	0	25	0	0
6	Z	28	0	25	0	0
6	a	28	0	25	0	0
7	R	39	0	34	0	0
7	V	39	0	34	0	0
7	W	39	0	34	1	0
8	A	56	0	52	0	0
8	B	56	0	52	2	0
8	C	28	0	26	1	0
All	All	18289	0	17499	218	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 6.

The worst 5 of 218 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:103:ILE:HG13	1:C:548:LEU:HD13	1.69	0.73
1:A:137:THR:HG22	1:A:258:ARG:HG2	1.71	0.71
1:A:173:MET:HA	1:A:176:ILE:HD12	1.71	0.71
1:A:140:VAL:HG23	1:A:255:THR:HG23	1.72	0.71
2:D:97:ASN:ND2	2:D:101:ASP:OD2	2.24	0.71

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	428/786 (54%)	411 (96%)	17 (4%)	0	100	100
1	B	411/786 (52%)	392 (95%)	19 (5%)	0	100	100
1	C	426/786 (54%)	410 (96%)	16 (4%)	0	100	100
2	D	116/224 (52%)	110 (95%)	5 (4%)	1 (1%)	14	41
2	G	116/224 (52%)	110 (95%)	6 (5%)	0	100	100
2	J	116/224 (52%)	112 (97%)	4 (3%)	0	100	100
3	E	104/214 (49%)	102 (98%)	2 (2%)	0	100	100
3	F	104/214 (49%)	100 (96%)	4 (4%)	0	100	100
3	I	104/214 (49%)	101 (97%)	3 (3%)	0	100	100
4	H	107/216 (50%)	101 (94%)	6 (6%)	0	100	100
5	K	128/234 (55%)	127 (99%)	1 (1%)	0	100	100
All	All	2160/4122 (52%)	2076 (96%)	83 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	100(A)	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/695 (58%)	396 (98%)	6 (2%)	60	76
1	B	387/695 (56%)	381 (98%)	6 (2%)	58	75
1	C	400/695 (58%)	397 (99%)	3 (1%)	79	87
2	D	102/194 (53%)	101 (99%)	1 (1%)	73	83
2	G	102/194 (53%)	102 (100%)	0	100	100
2	J	102/194 (53%)	102 (100%)	0	100	100
3	E	89/182 (49%)	88 (99%)	1 (1%)	70	81
3	F	89/182 (49%)	89 (100%)	0	100	100
3	I	89/182 (49%)	89 (100%)	0	100	100
4	H	89/182 (49%)	89 (100%)	0	100	100
5	K	107/197 (54%)	105 (98%)	2 (2%)	52	71
All	All	1958/3592 (54%)	1939 (99%)	19 (1%)	71	83

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	548	LEU
5	K	39	GLN
5	K	82(B)	ARG
3	E	49	TYR
1	B	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
5	K	3	GLN
5	K	39	GLN
1	C	319	HIS
1	C	202	HIS
5	K	100(G)	ASN

5.3.3 RNA

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)

35 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	$\#\|Z\| > 2$
6	NAG	L	1	1,6	14,14,15	0.71	0	17,19,21	1.11	1 (5%)
6	NAG	L	2	6	14,14,15	0.68	0	17,19,21	1.18	1 (5%)
6	NAG	M	1	1,6	14,14,15	0.73	0	17,19,21	0.82	0
6	NAG	M	2	6	14,14,15	0.69	0	17,19,21	0.83	0
6	NAG	N	1	1,6	14,14,15	0.72	0	17,19,21	0.85	0
6	NAG	N	2	6	14,14,15	0.69	0	17,19,21	0.89	0
6	NAG	O	1	1,6	14,14,15	0.72	0	17,19,21	0.86	0
6	NAG	O	2	6	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
6	NAG	P	1	1,6	14,14,15	0.75	0	17,19,21	0.91	0
6	NAG	P	2	6	14,14,15	0.72	0	17,19,21	1.21	1 (5%)
6	NAG	Q	1	1,6	14,14,15	0.67	0	17,19,21	1.37	2 (11%)
6	NAG	Q	2	6	14,14,15	0.73	0	17,19,21	1.18	1 (5%)
7	NAG	R	1	1,7	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
7	NAG	R	2	7	14,14,15	0.71	0	17,19,21	0.89	0
7	BMA	R	3	7	11,11,12	0.84	0	15,15,17	2.58	6 (40%)
6	NAG	S	1	1,6	14,14,15	0.69	0	17,19,21	1.26	1 (5%)
6	NAG	S	2	6	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
6	NAG	T	1	1,6	14,14,15	0.70	0	17,19,21	1.19	1 (5%)
6	NAG	T	2	6	14,14,15	0.70	0	17,19,21	1.20	1 (5%)
6	NAG	U	1	1,6	14,14,15	0.76	0	17,19,21	0.89	0
6	NAG	U	2	6	14,14,15	0.72	0	17,19,21	0.84	0
7	NAG	V	1	1,7	14,14,15	0.77	0	17,19,21	0.95	1 (5%)
7	NAG	V	2	7	14,14,15	0.71	0	17,19,21	0.99	0
7	BMA	V	3	7	11,11,12	0.81	0	15,15,17	2.82	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	W	1	1,7	14,14,15	0.70	0	17,19,21	0.81	0
7	NAG	W	2	7	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
7	BMA	W	3	7	11,11,12	0.83	0	15,15,17	2.70	7 (46%)
6	NAG	X	1	1,6	14,14,15	0.71	0	17,19,21	0.85	0
6	NAG	X	2	6	14,14,15	0.72	0	17,19,21	0.85	0
6	NAG	Y	1	1,6	14,14,15	0.71	0	17,19,21	0.87	0
6	NAG	Y	2	6	14,14,15	0.72	0	17,19,21	0.79	0
6	NAG	Z	1	1,6	14,14,15	0.72	0	17,19,21	0.89	0
6	NAG	Z	2	6	14,14,15	0.70	0	17,19,21	1.23	1 (5%)
6	NAG	a	1	1,6	14,14,15	0.72	0	17,19,21	1.17	1 (5%)
6	NAG	a	2	6	14,14,15	0.71	0	17,19,21	0.87	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
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1
6	NAG	M	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1
6	NAG	N	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	4/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	4/6/23/26	0/1/1/1
7	NAG	R	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	V	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	1/6/23/26	0/1/1/1
7	BMA	V	3	7	-	0/2/19/22	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
7	BMA	W	3	7	-	0/2/19/22	0/1/1/1
6	NAG	X	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	X	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Y	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	3/6/23/26	0/1/1/1
6	NAG	Z	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	3	BMA	C1-O5-C5	8.38	123.42	112.19
7	W	3	BMA	C1-O5-C5	7.84	122.69	112.19
7	R	3	BMA	C1-O5-C5	7.19	121.82	112.19
6	Q	1	NAG	C2-N2-C7	4.00	128.26	122.90
7	R	3	BMA	C3-C4-C5	3.74	117.01	110.23

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	2	NAG	C4-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6

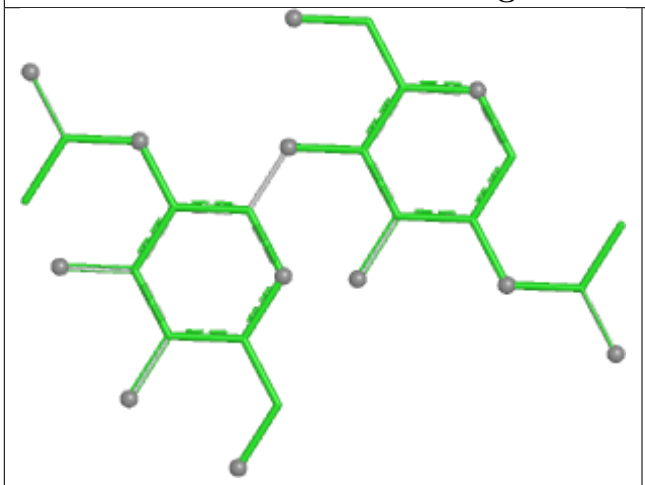
There are no ring outliers.

3 monomers are involved in 3 short contacts:

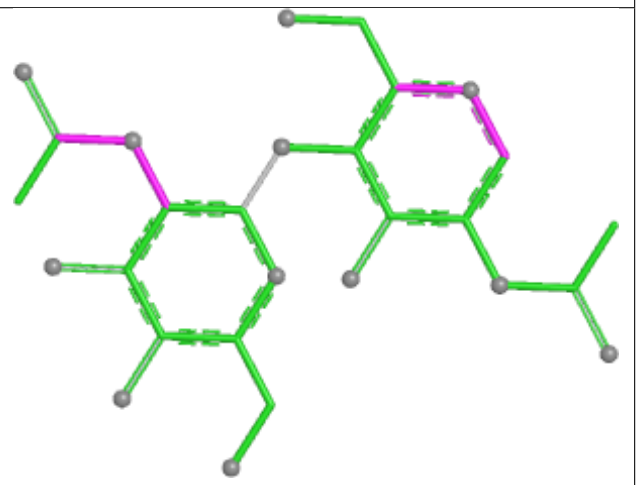
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	W	1	NAG	1	0
6	X	2	NAG	1	0
6	Q	1	NAG	1	0

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

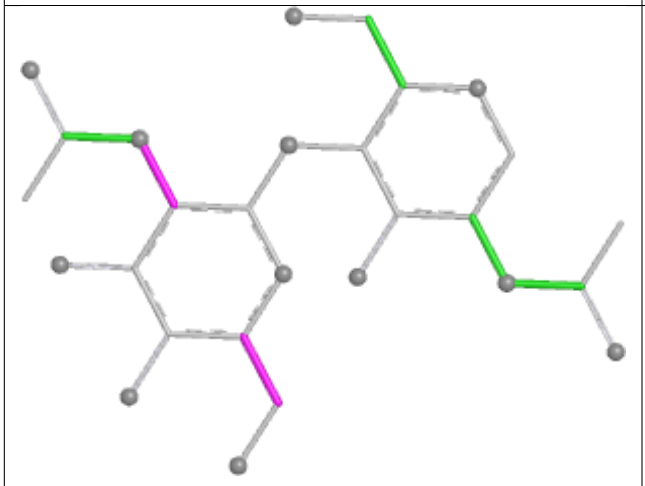
Oligosaccharide Chain L



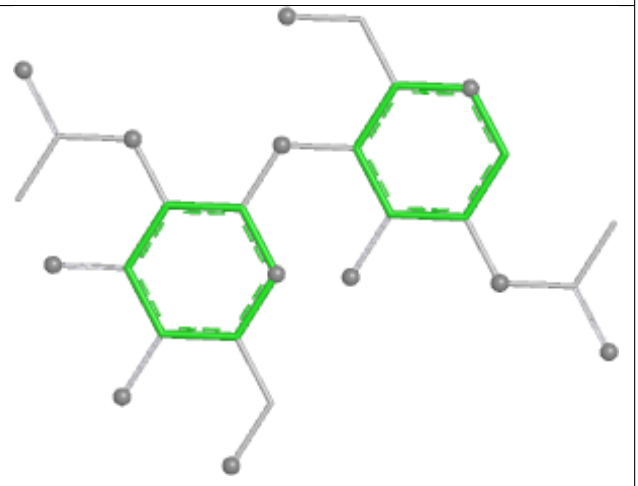
Bond lengths



Bond angles

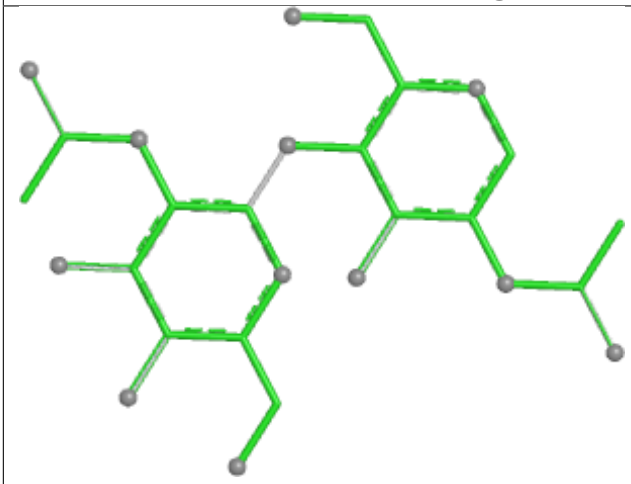


Torsions

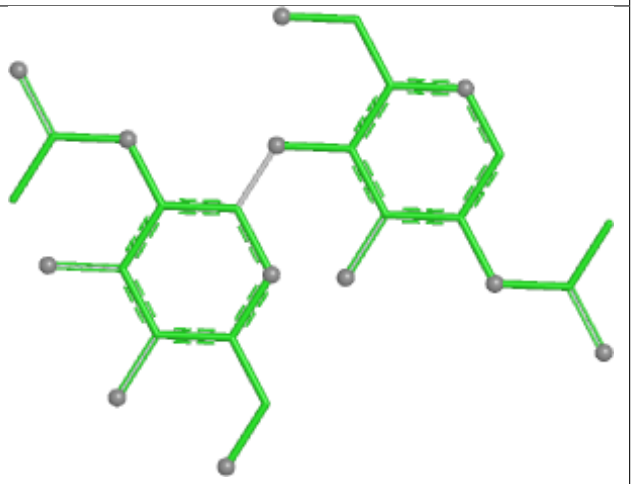


Rings

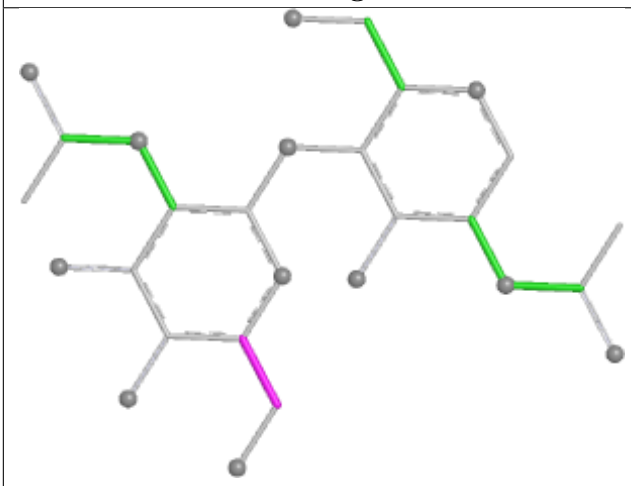
Oligosaccharide Chain M



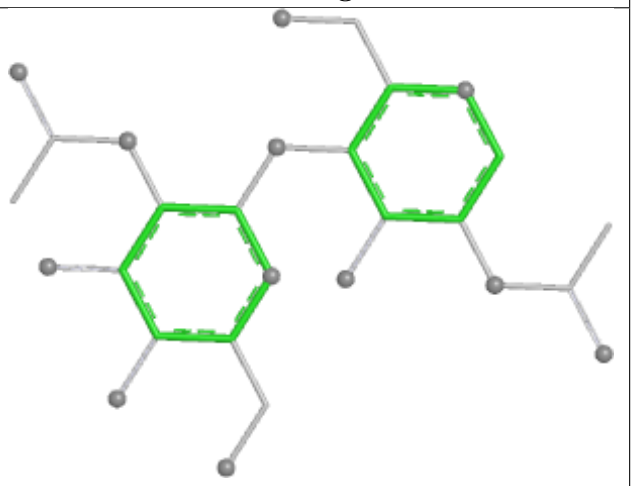
Bond lengths



Bond angles

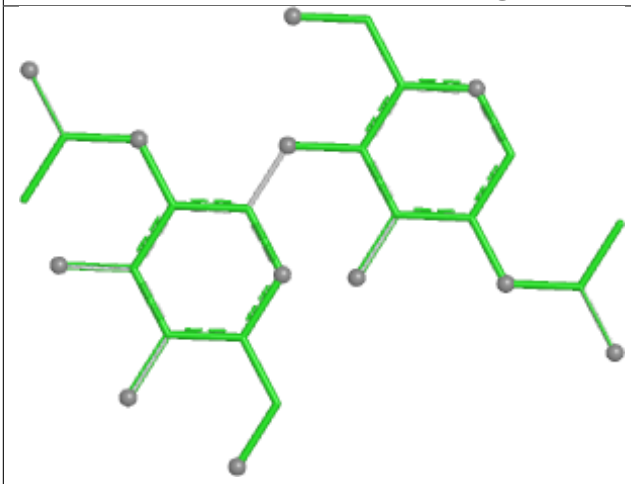


Torsions

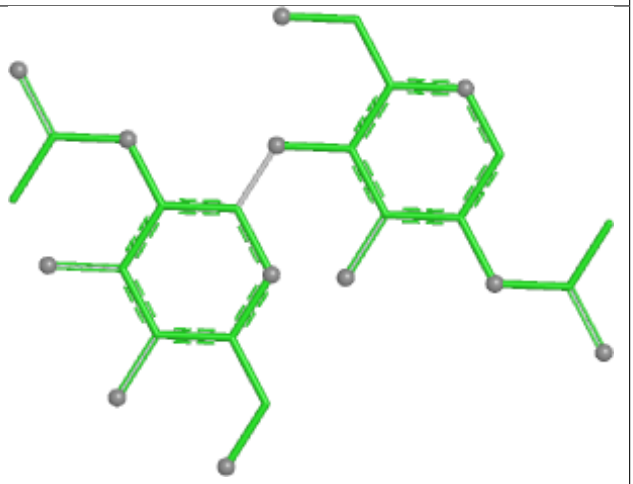


Rings

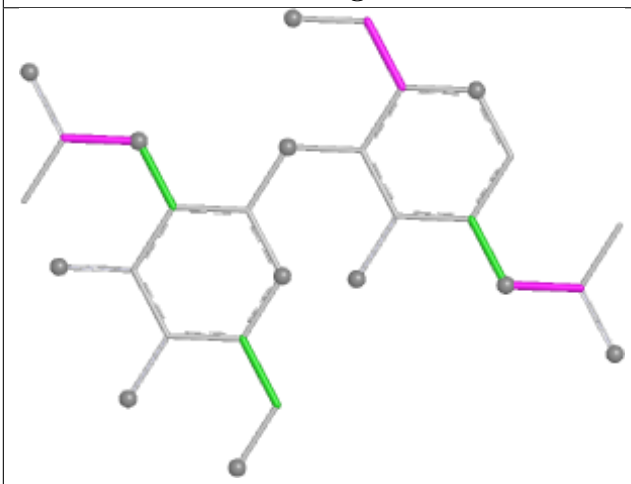
Oligosaccharide Chain N



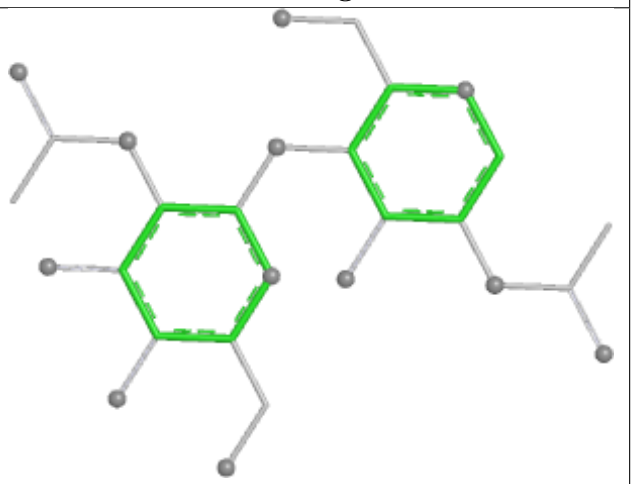
Bond lengths



Bond angles

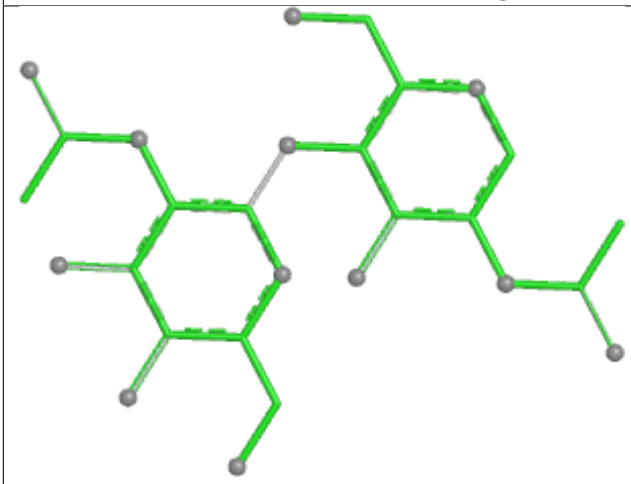


Torsions

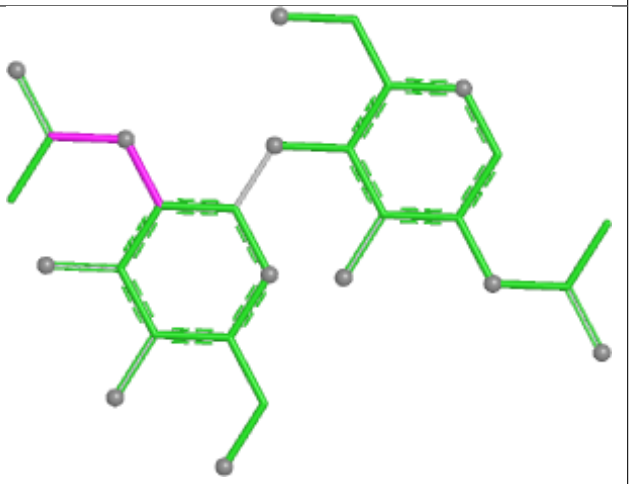


Rings

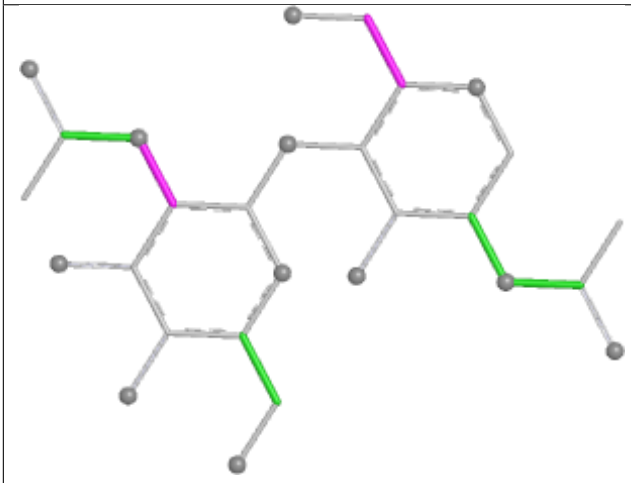
Oligosaccharide Chain O



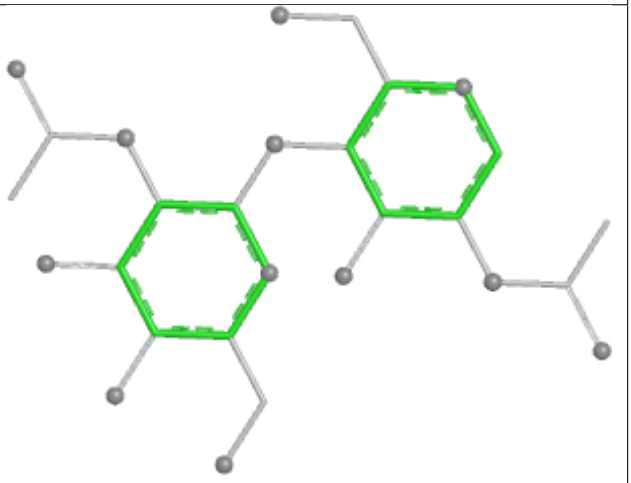
Bond lengths



Bond angles

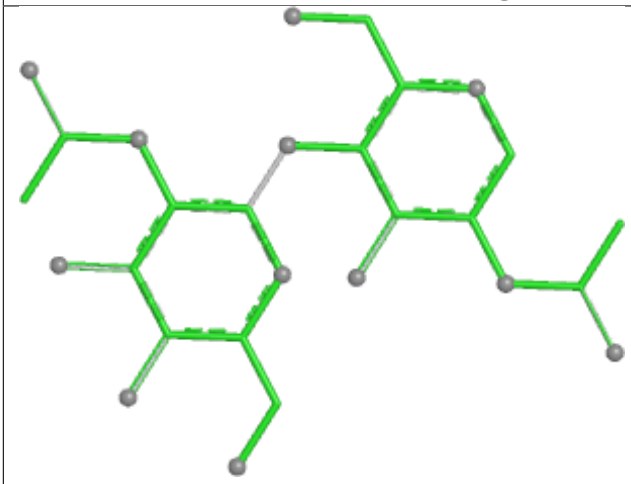


Torsions

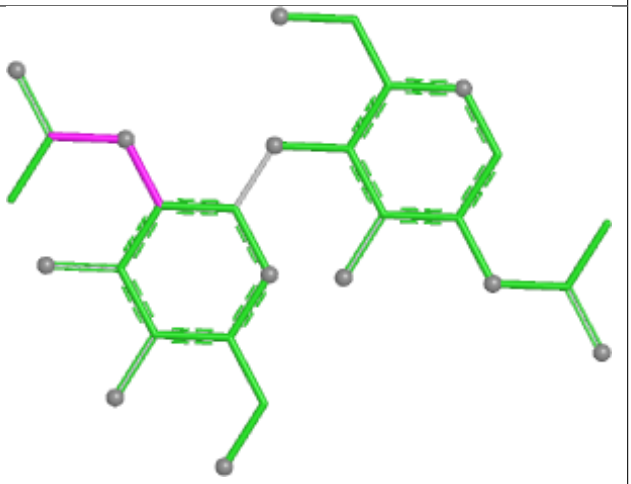


Rings

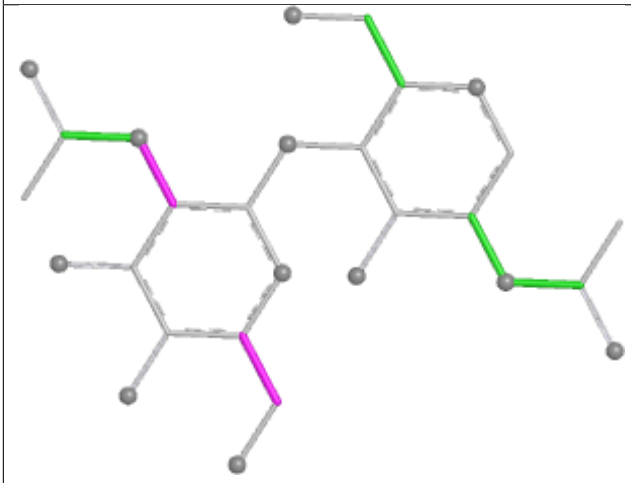
Oligosaccharide Chain P



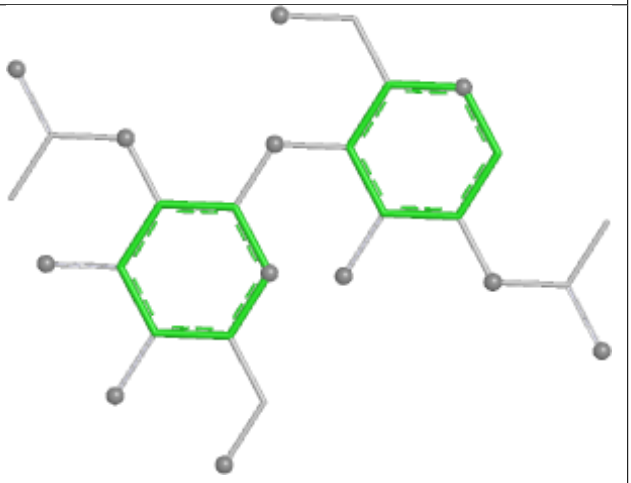
Bond lengths



Bond angles

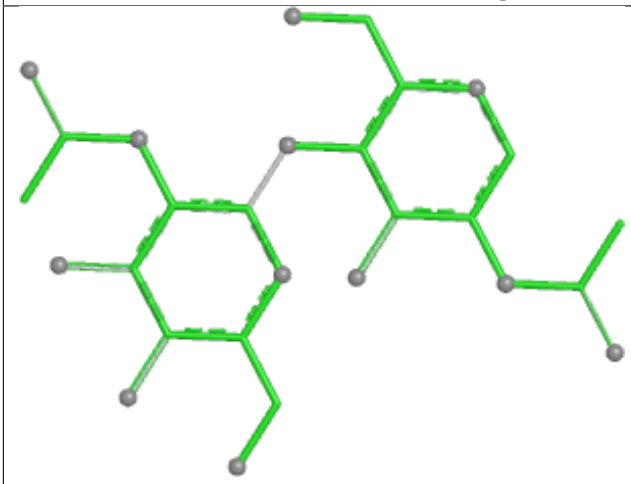


Torsions

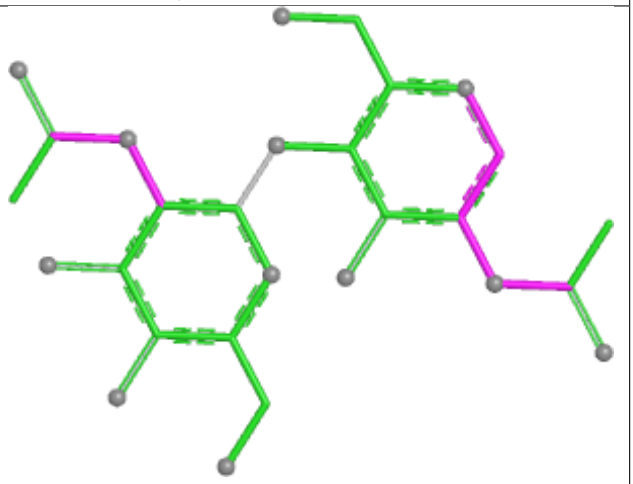


Rings

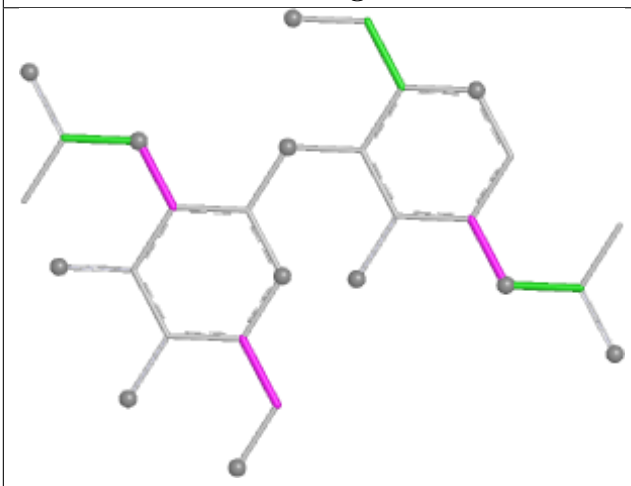
Oligosaccharide Chain Q



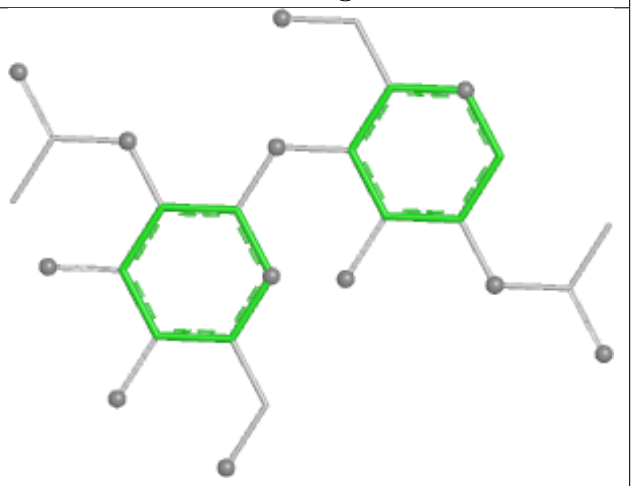
Bond lengths



Bond angles

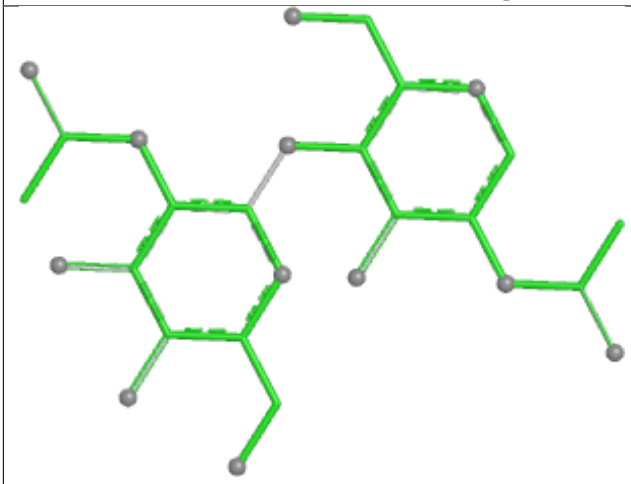


Torsions

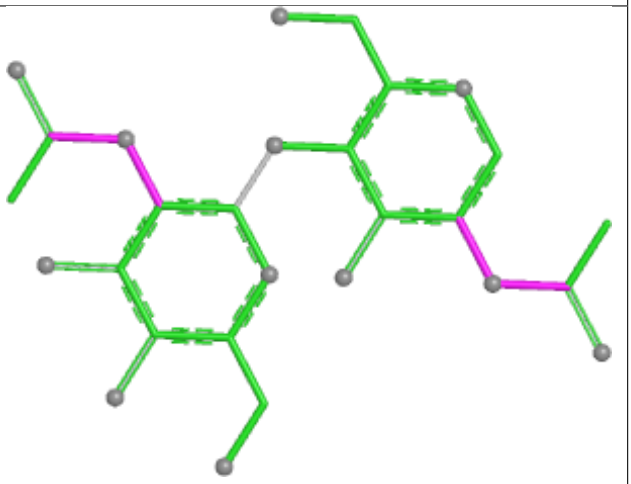


Rings

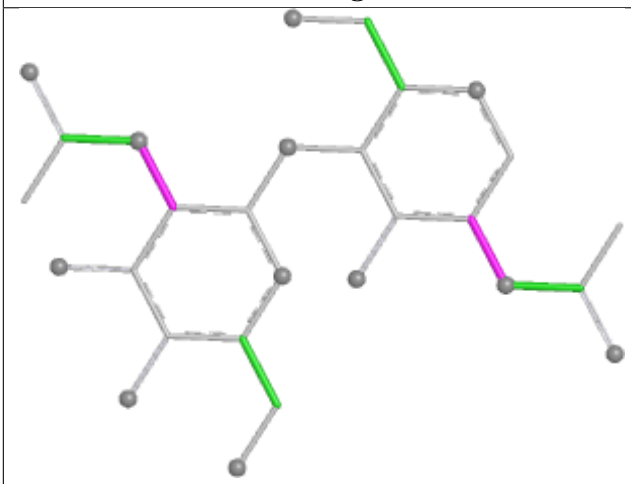
Oligosaccharide Chain S



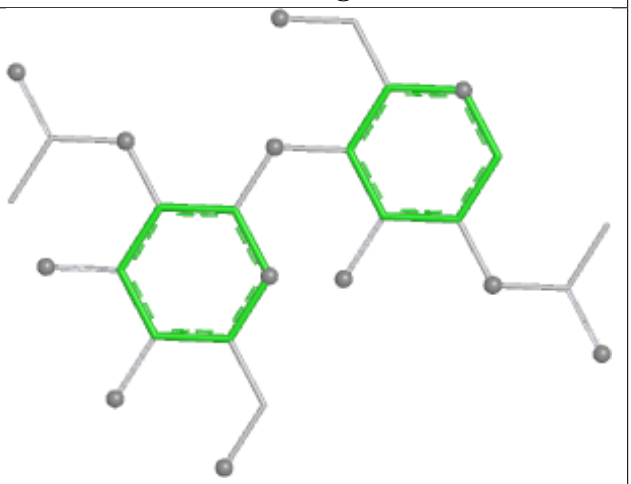
Bond lengths



Bond angles

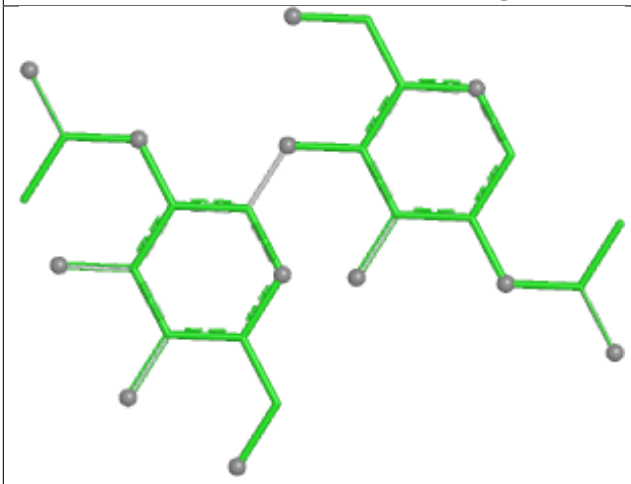


Torsions

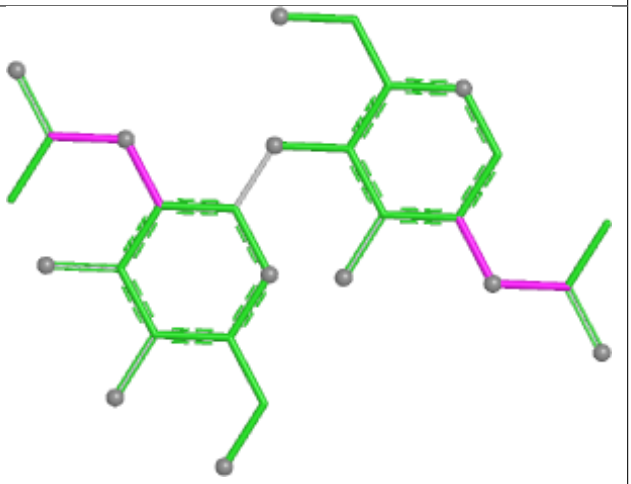


Rings

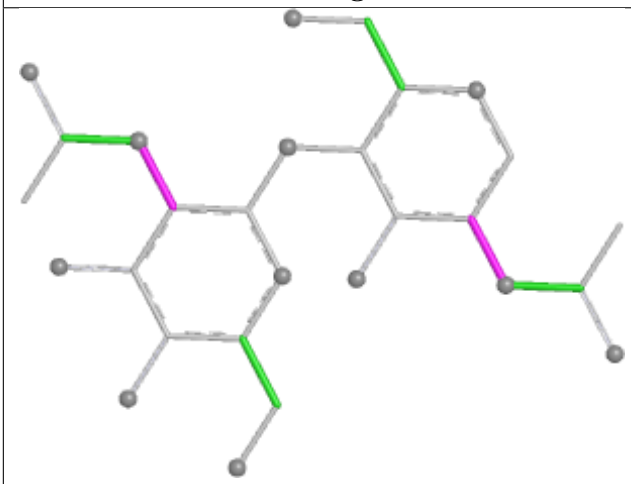
Oligosaccharide Chain T



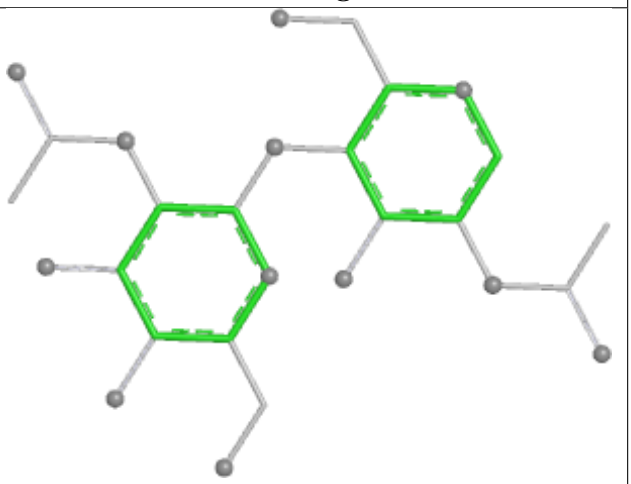
Bond lengths



Bond angles

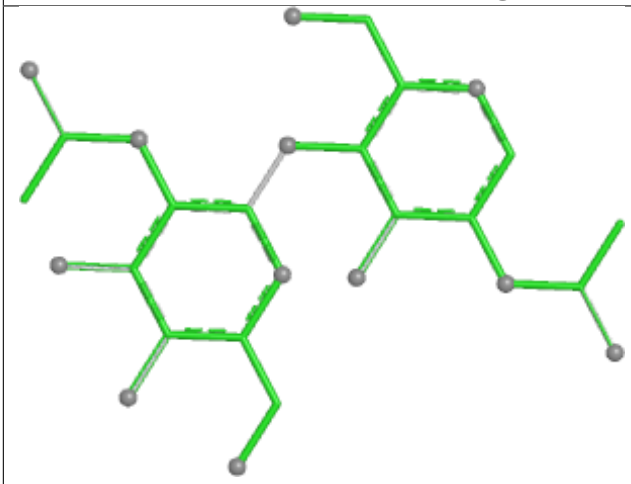


Torsions

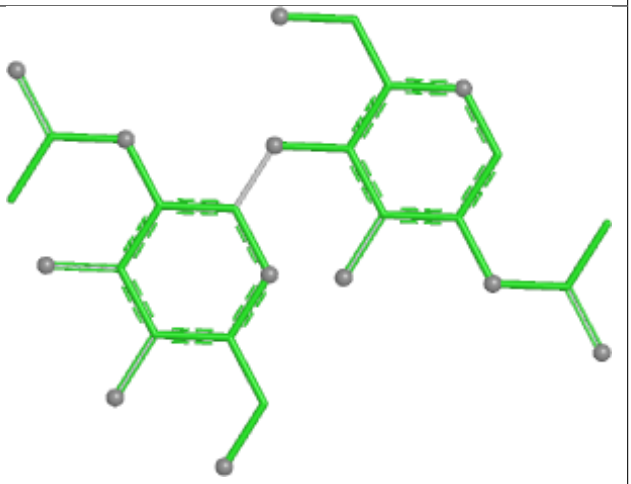


Rings

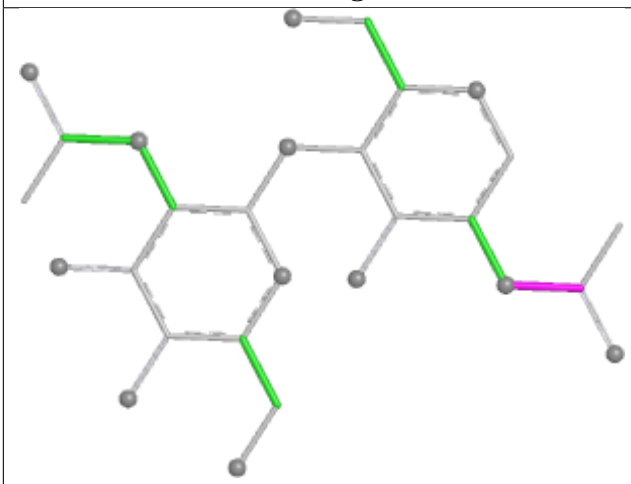
Oligosaccharide Chain U



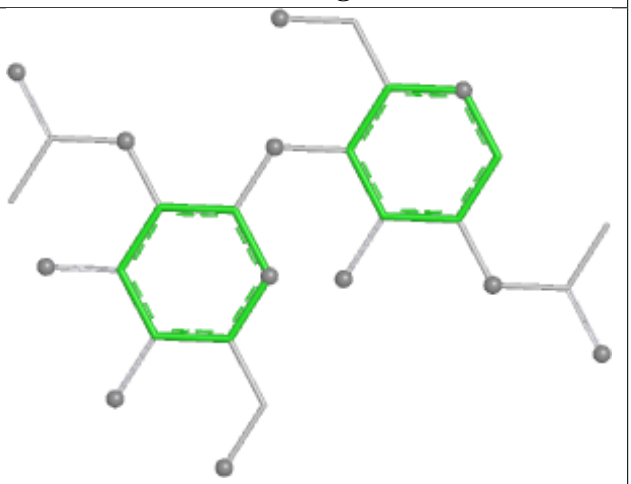
Bond lengths



Bond angles

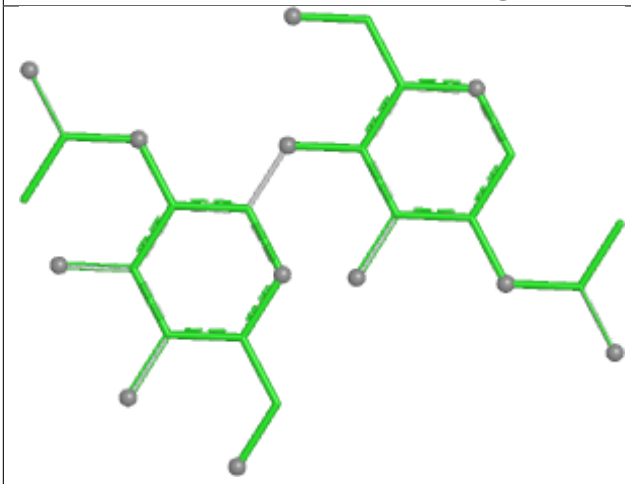


Torsions

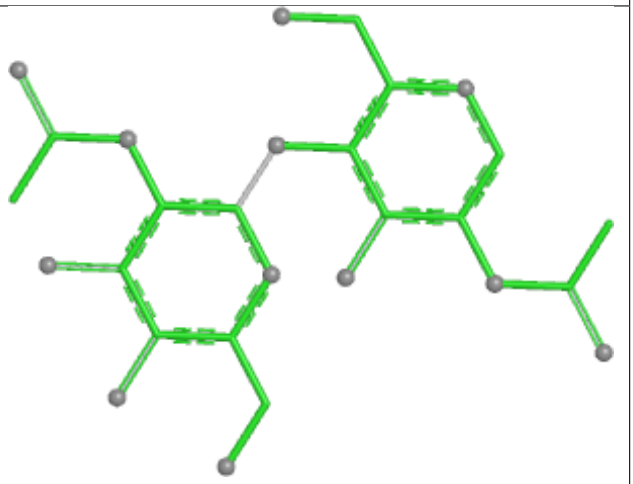


Rings

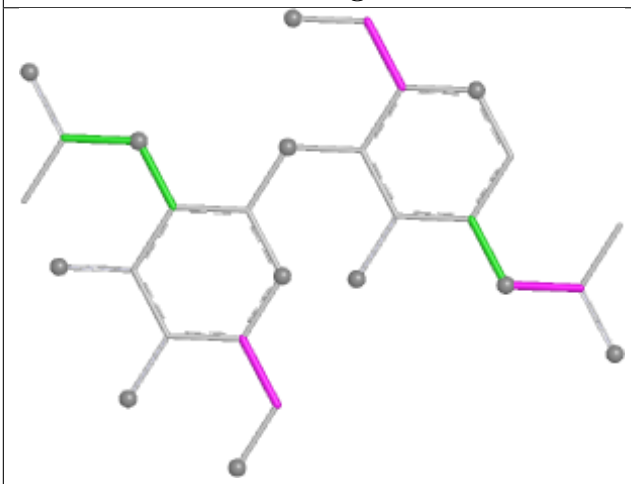
Oligosaccharide Chain X



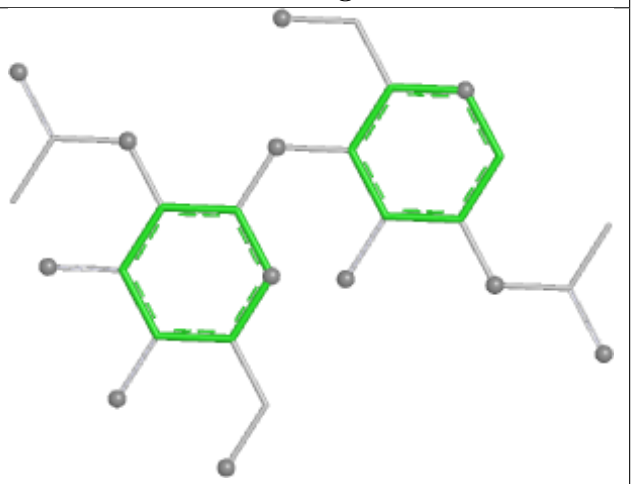
Bond lengths



Bond angles

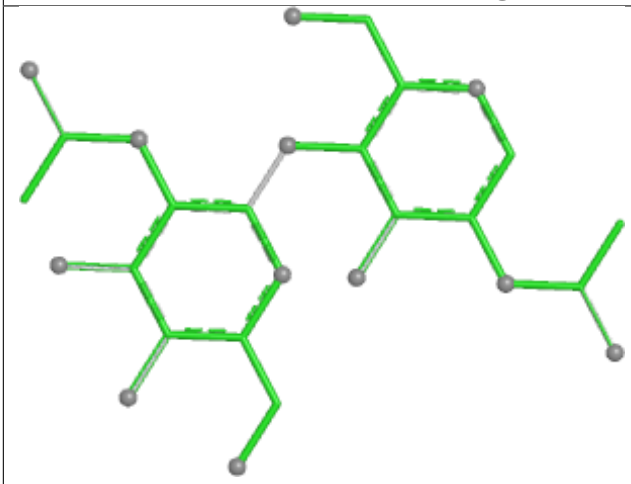


Torsions

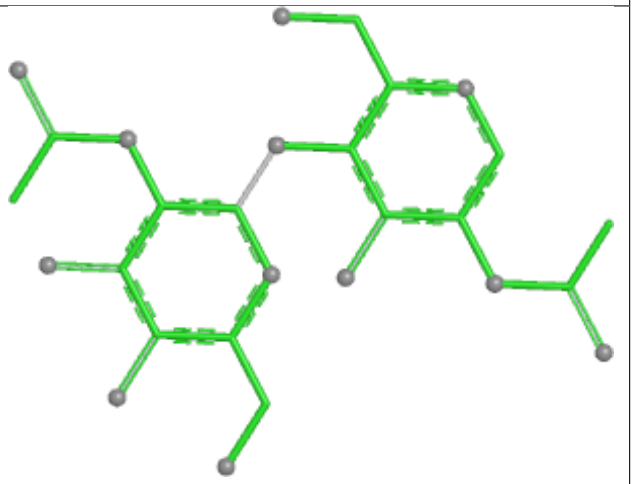


Rings

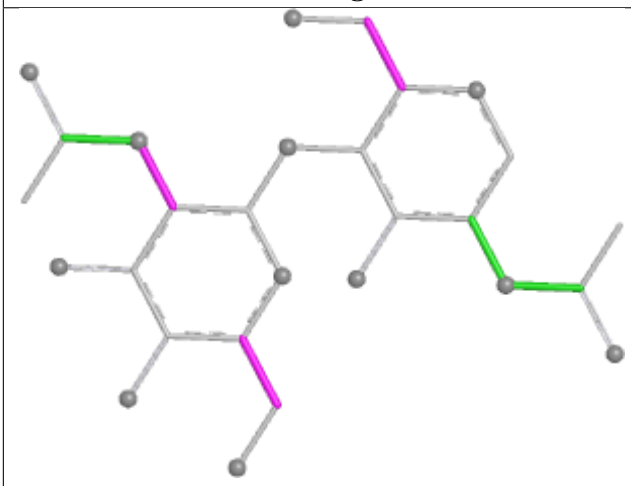
Oligosaccharide Chain Y



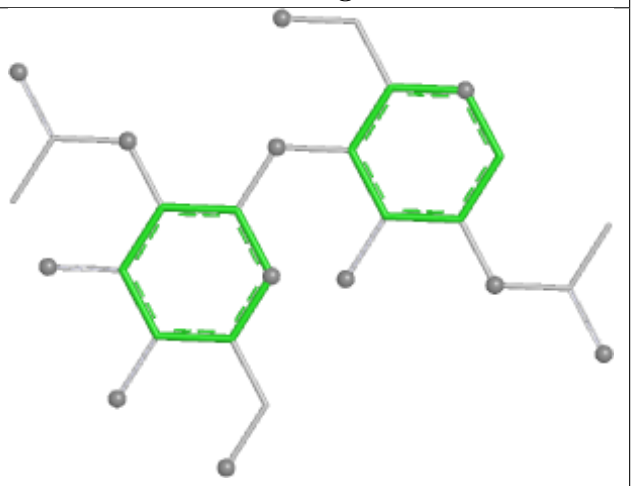
Bond lengths



Bond angles

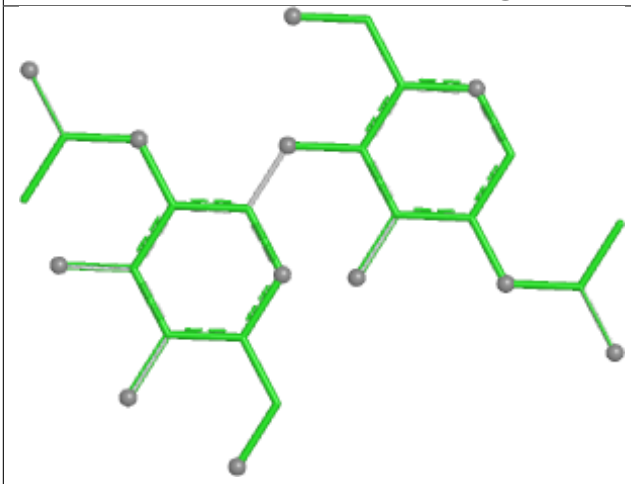


Torsions

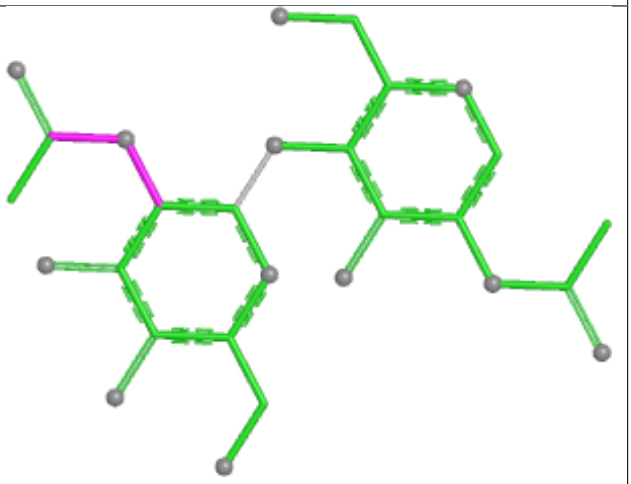


Rings

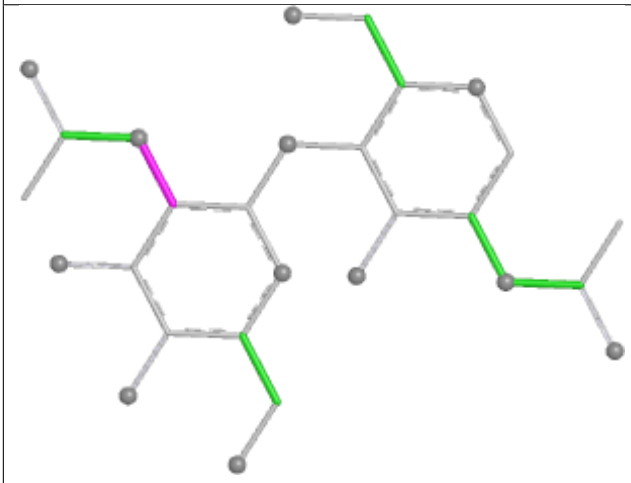
Oligosaccharide Chain Z



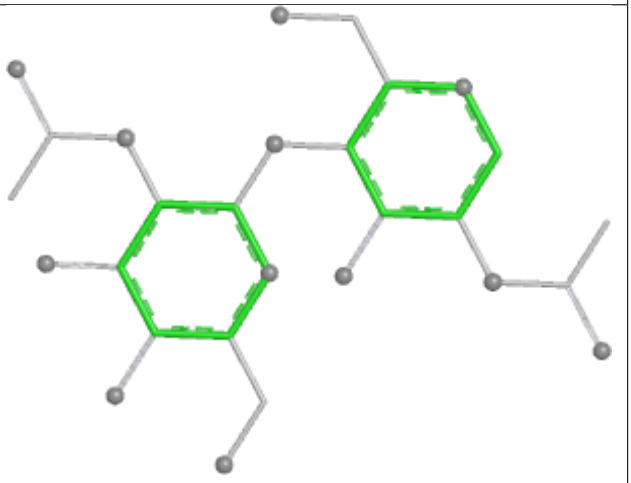
Bond lengths



Bond angles

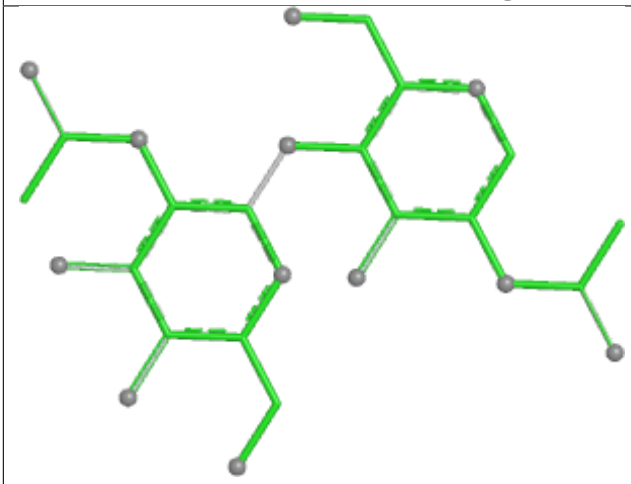


Torsions

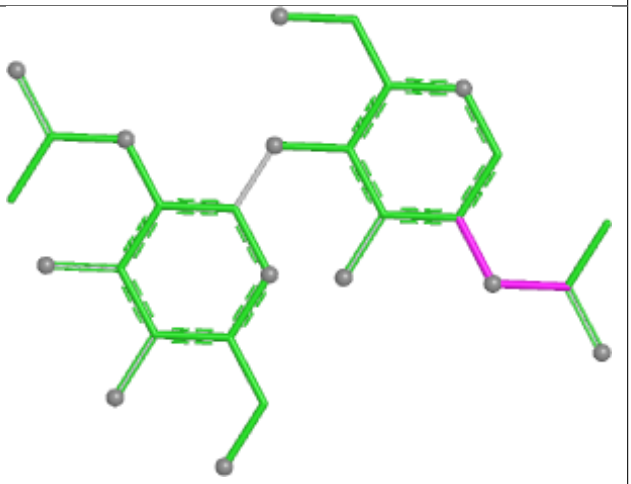


Rings

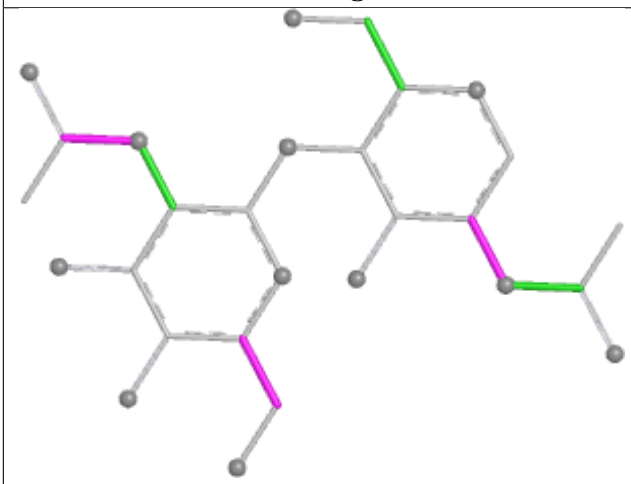
Oligosaccharide Chain a



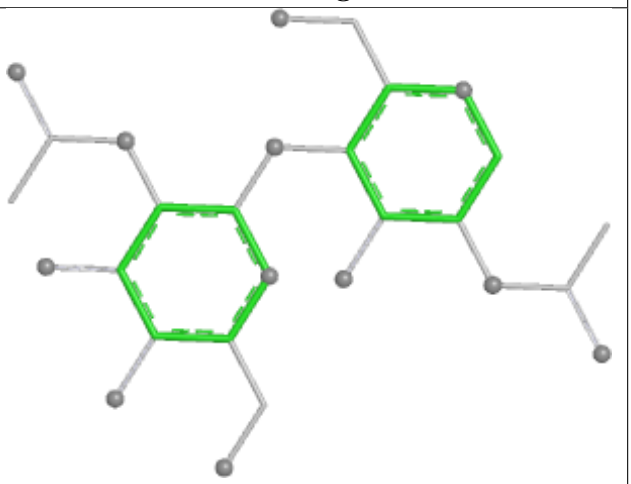
Bond lengths



Bond angles

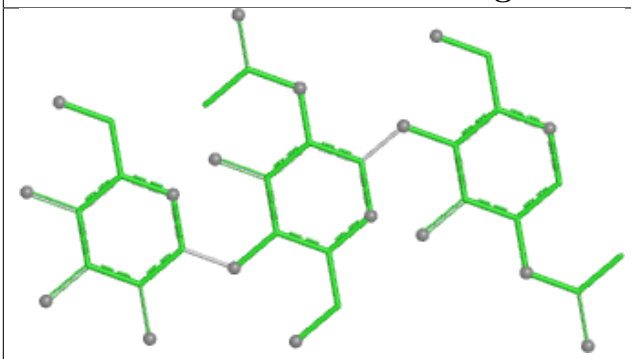


Torsions

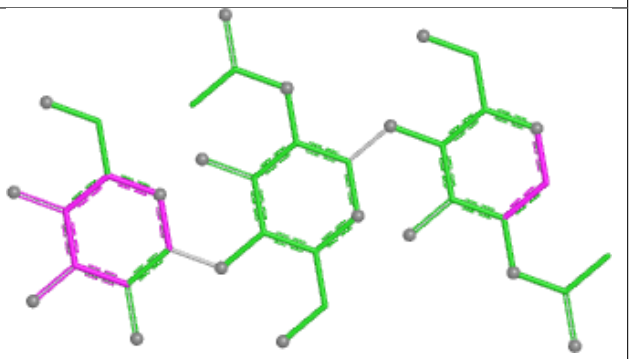


Rings

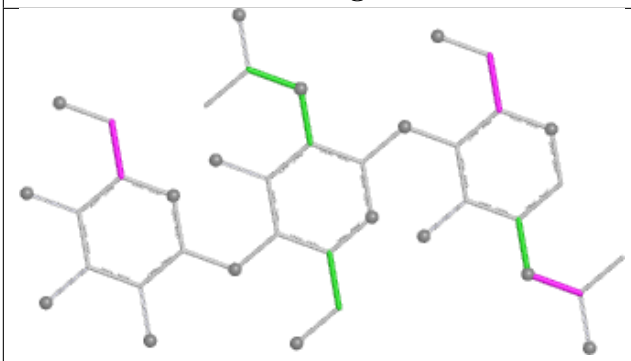
Oligosaccharide Chain R



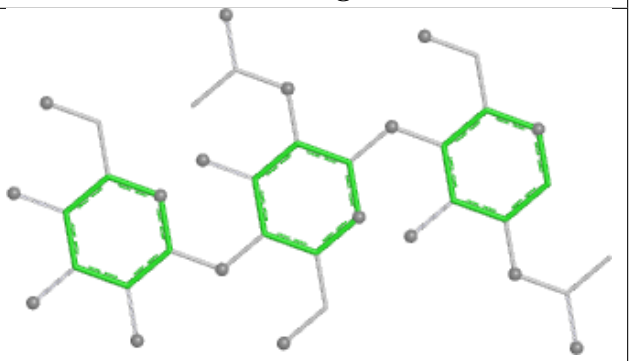
Bond lengths



Bond angles

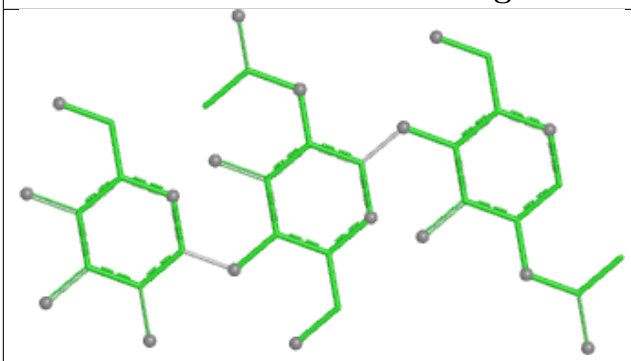


Torsions

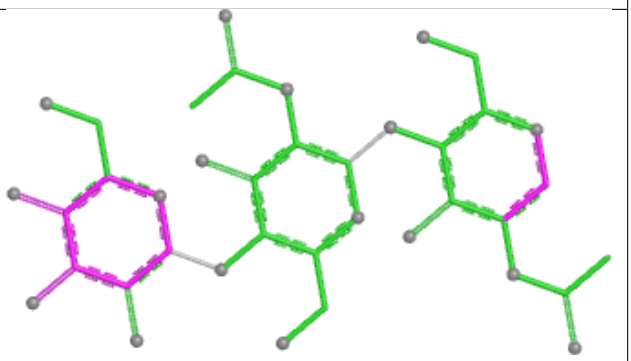


Rings

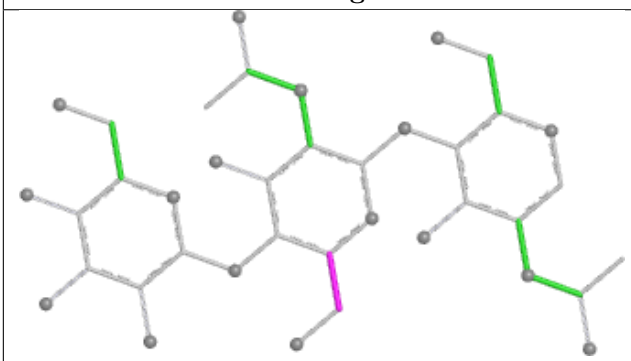
Oligosaccharide Chain V



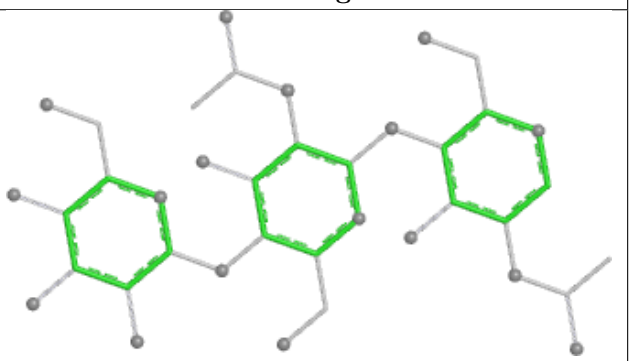
Bond lengths



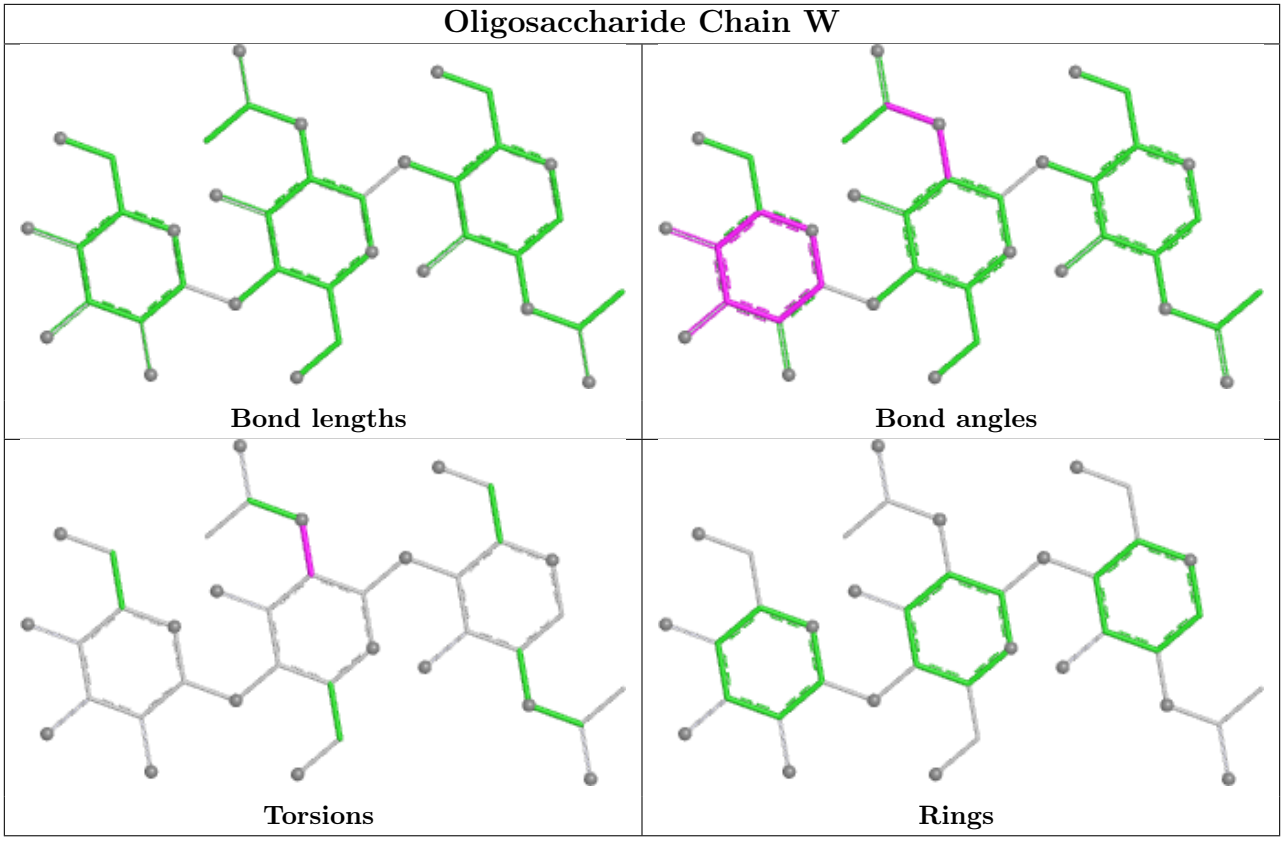
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

10 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	A	801	1	14,14,15	0.70	0	17,19,21	1.16	1 (5%)
8	NAG	C	801	1	14,14,15	0.68	0	17,19,21	0.85	0
8	NAG	B	803	1	14,14,15	0.71	0	17,19,21	0.85	0
8	NAG	A	803	1	14,14,15	0.70	0	17,19,21	0.94	0
8	NAG	B	802	1	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
8	NAG	C	802	1	14,14,15	0.74	0	17,19,21	1.12	1 (5%)
8	NAG	A	804	1	14,14,15	0.70	0	17,19,21	0.90	0
8	NAG	B	804	1	14,14,15	0.69	0	17,19,21	0.89	0
8	NAG	B	801	1	14,14,15	0.70	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	802	1	14,14,15	0.71	0	17,19,21	0.84	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
8	NAG	A	801	1	-	4/6/23/26	0/1/1/1
8	NAG	C	801	1	-	4/6/23/26	0/1/1/1
8	NAG	B	803	1	-	2/6/23/26	0/1/1/1
8	NAG	A	803	1	-	3/6/23/26	0/1/1/1
8	NAG	B	802	1	-	2/6/23/26	0/1/1/1
8	NAG	C	802	1	-	2/6/23/26	0/1/1/1
8	NAG	A	804	1	-	4/6/23/26	0/1/1/1
8	NAG	B	804	1	-	2/6/23/26	0/1/1/1
8	NAG	B	801	1	-	1/6/23/26	0/1/1/1
8	NAG	A	802	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	802	NAG	C2-N2-C7	3.27	127.28	122.90
8	C	802	NAG	C2-N2-C7	3.19	127.17	122.90
8	A	801	NAG	C2-N2-C7	3.13	127.09	122.90

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	803	NAG	C4-C5-C6-O6
8	A	801	NAG	O5-C5-C6-O6
8	B	803	NAG	O5-C5-C6-O6
8	C	801	NAG	C4-C5-C6-O6
8	A	804	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	803	NAG	2	0
8	C	802	NAG	1	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.

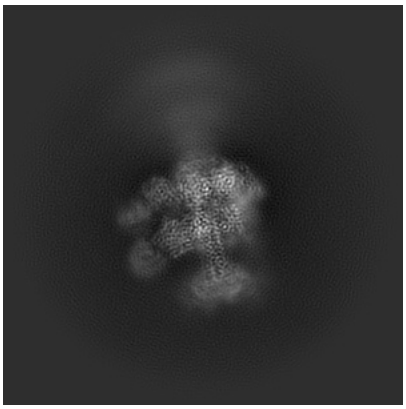
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43667. These allow visual inspection of the internal detail of the map and identification of artifacts.

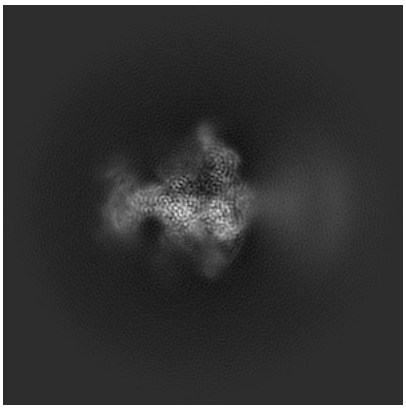
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

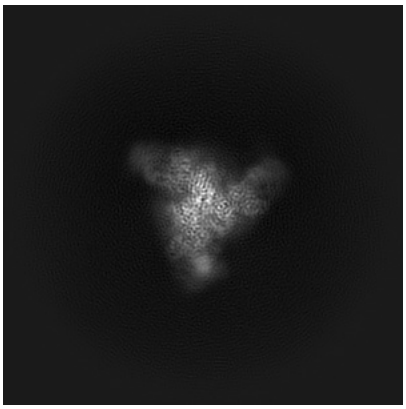
6.1.1 Primary map



X

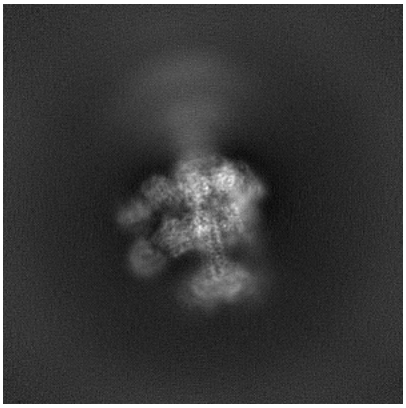


Y

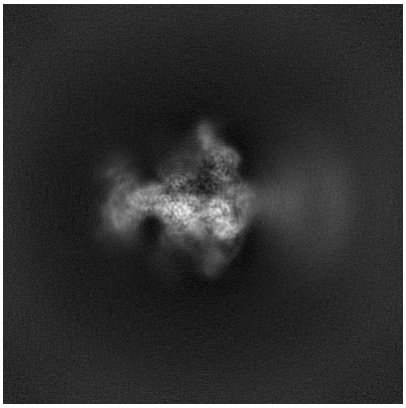


Z

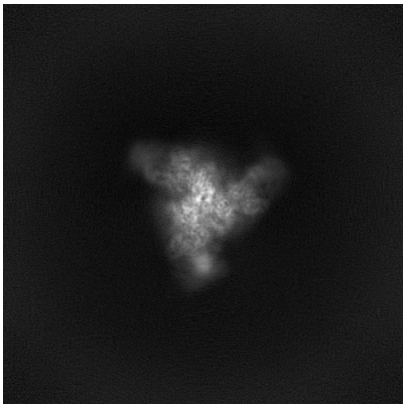
6.1.2 Raw map



X



Y

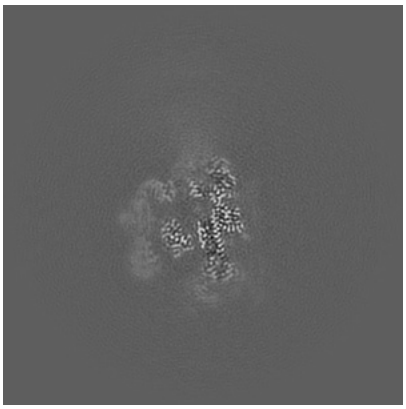


Z

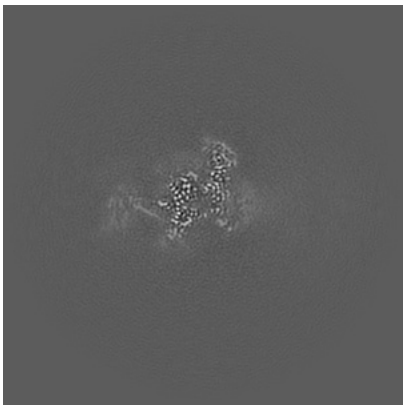
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

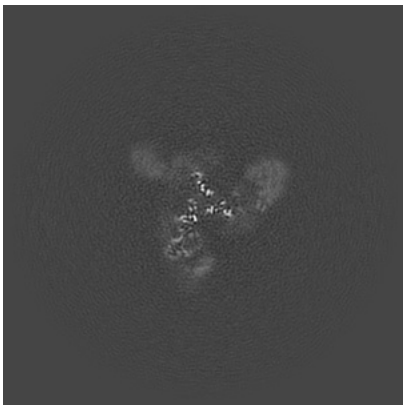
6.2.1 Primary map



X Index: 256

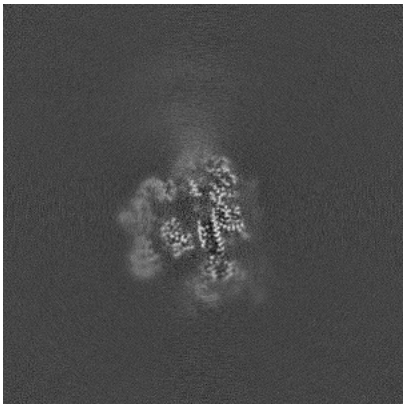


Y Index: 256

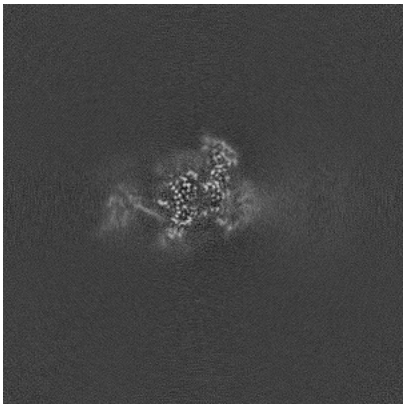


Z Index: 256

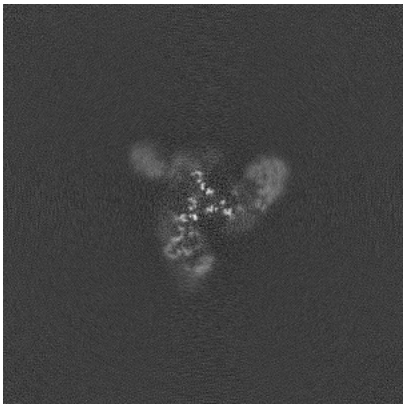
6.2.2 Raw map



X Index: 256



Y Index: 256

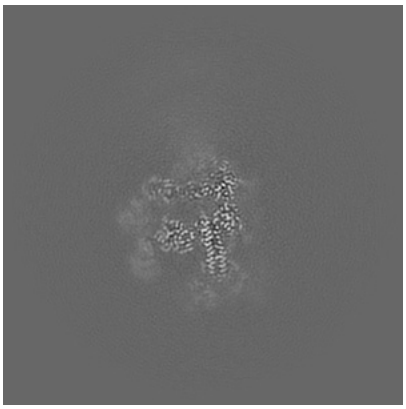


Z Index: 256

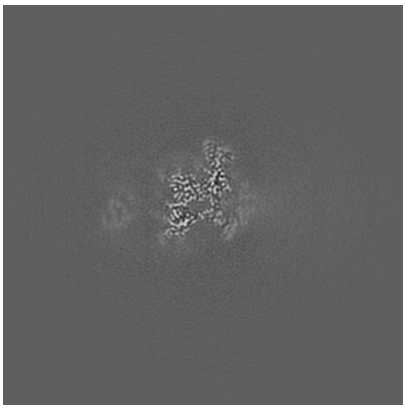
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

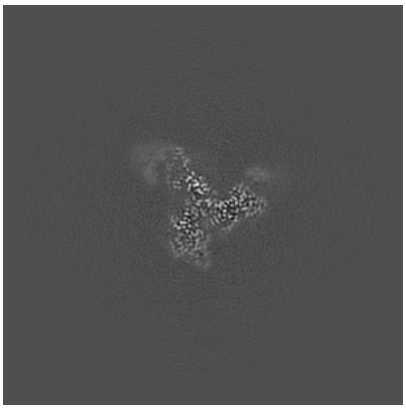
6.3.1 Primary map



X Index: 251

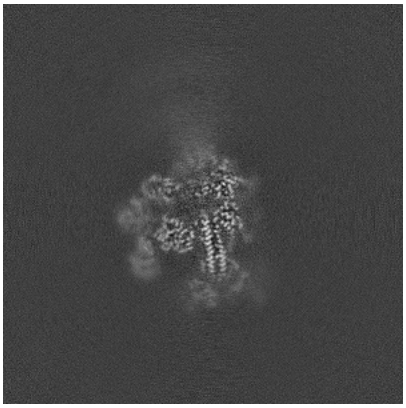


Y Index: 251

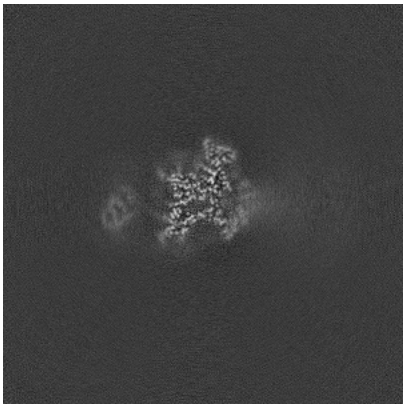


Z Index: 275

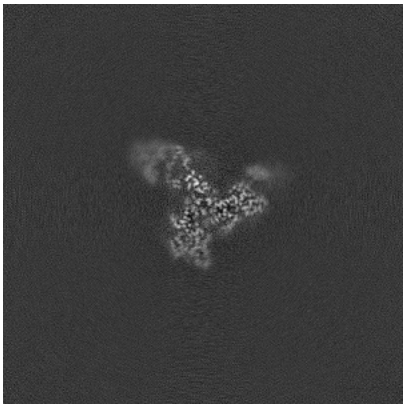
6.3.2 Raw map



X Index: 251



Y Index: 250

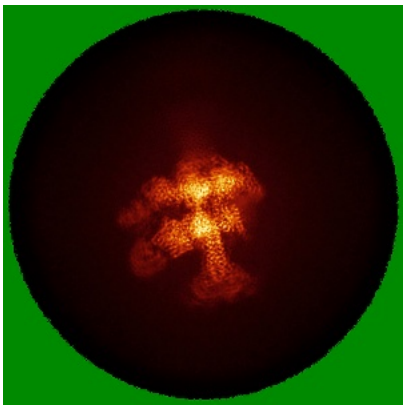


Z Index: 275

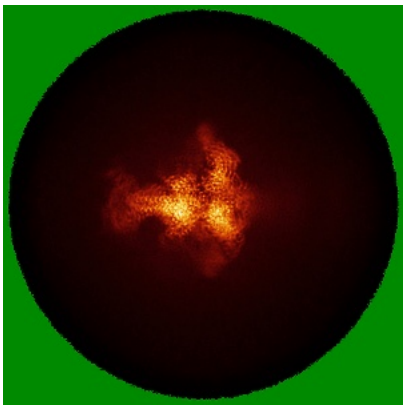
The images above show the largest variance slices of the map in three orthogonal directions.

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

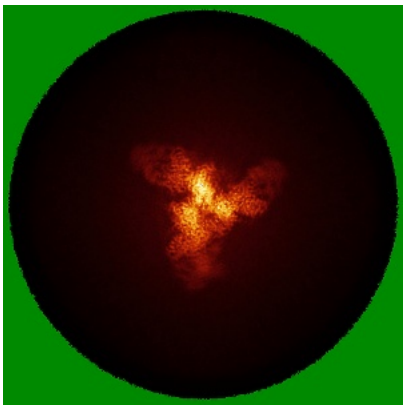
6.4.1 Primary map



X

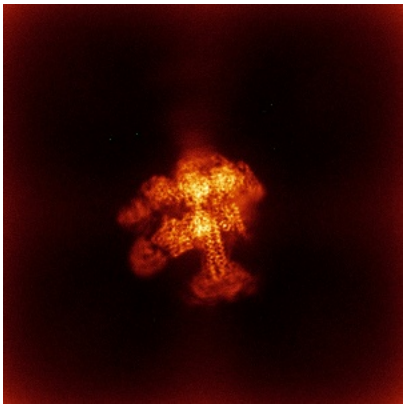


Y

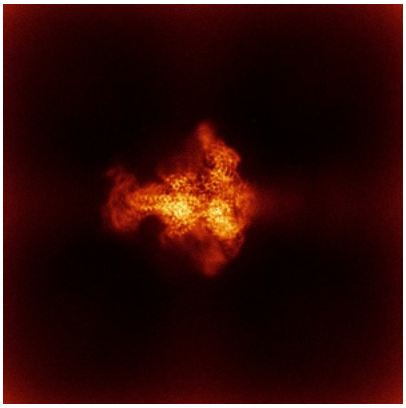


Z

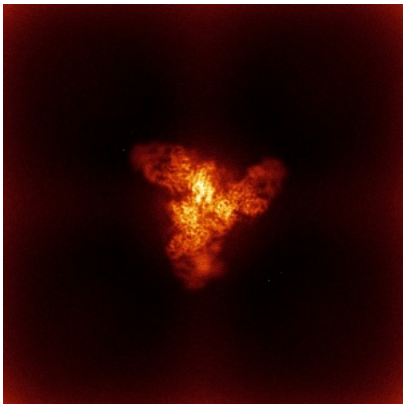
6.4.2 Raw map



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 0.17. 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.

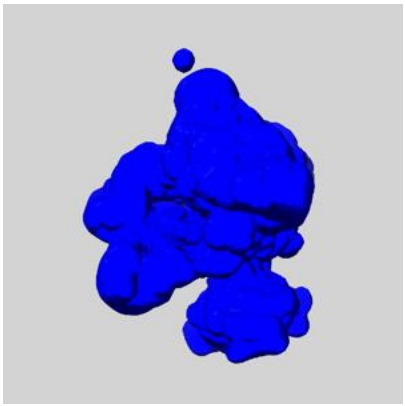
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

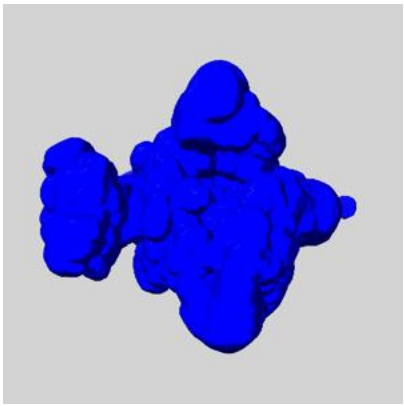
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

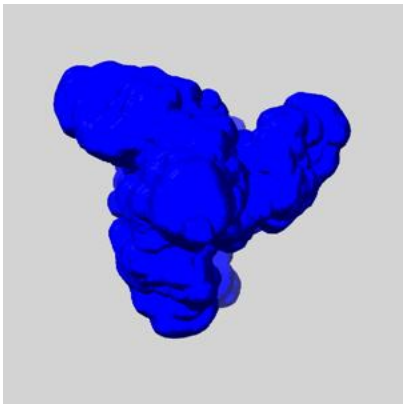
6.6.1 emd_43667_msk_1.map (i)



X



Y

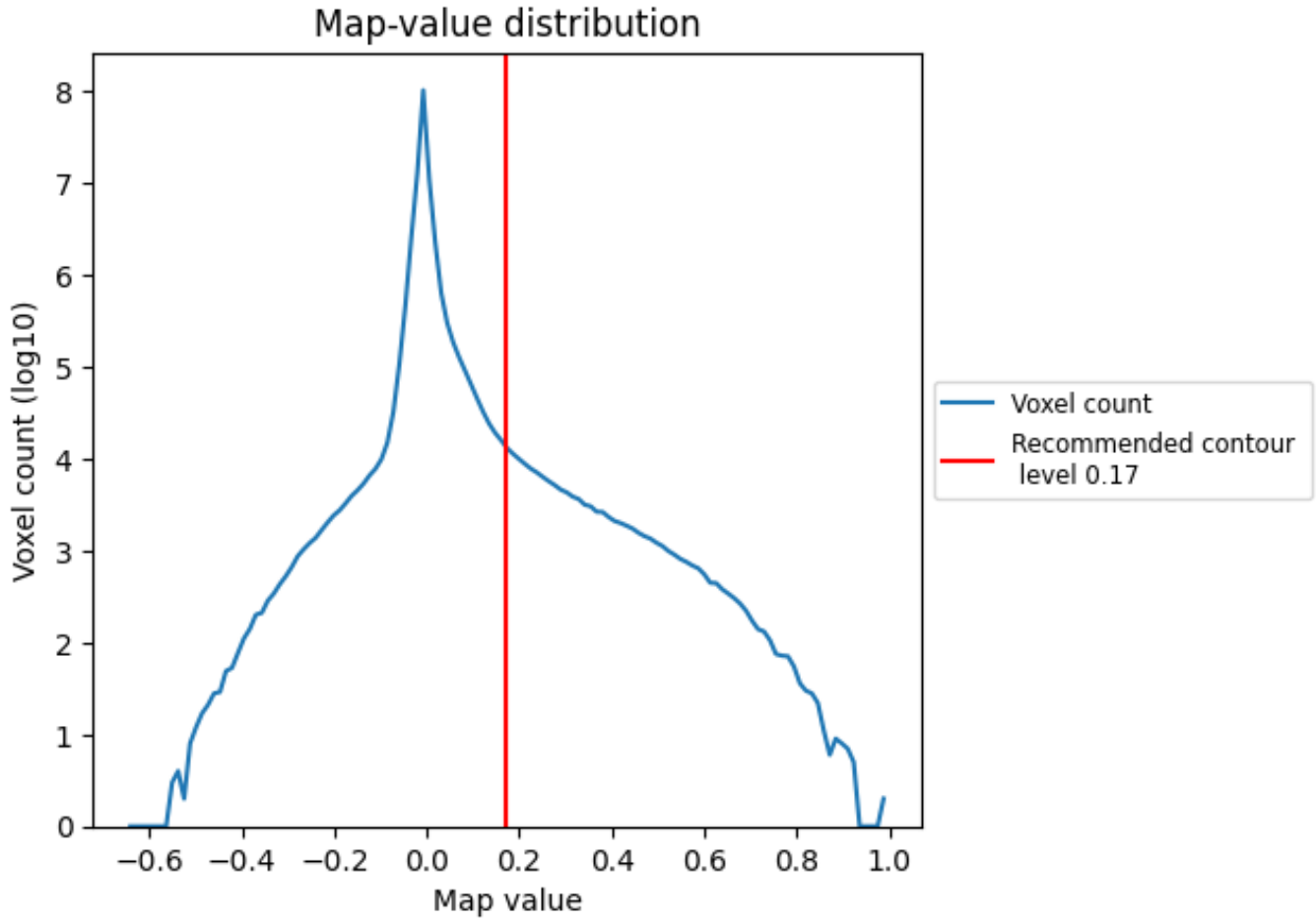


Z

7 Map analysis

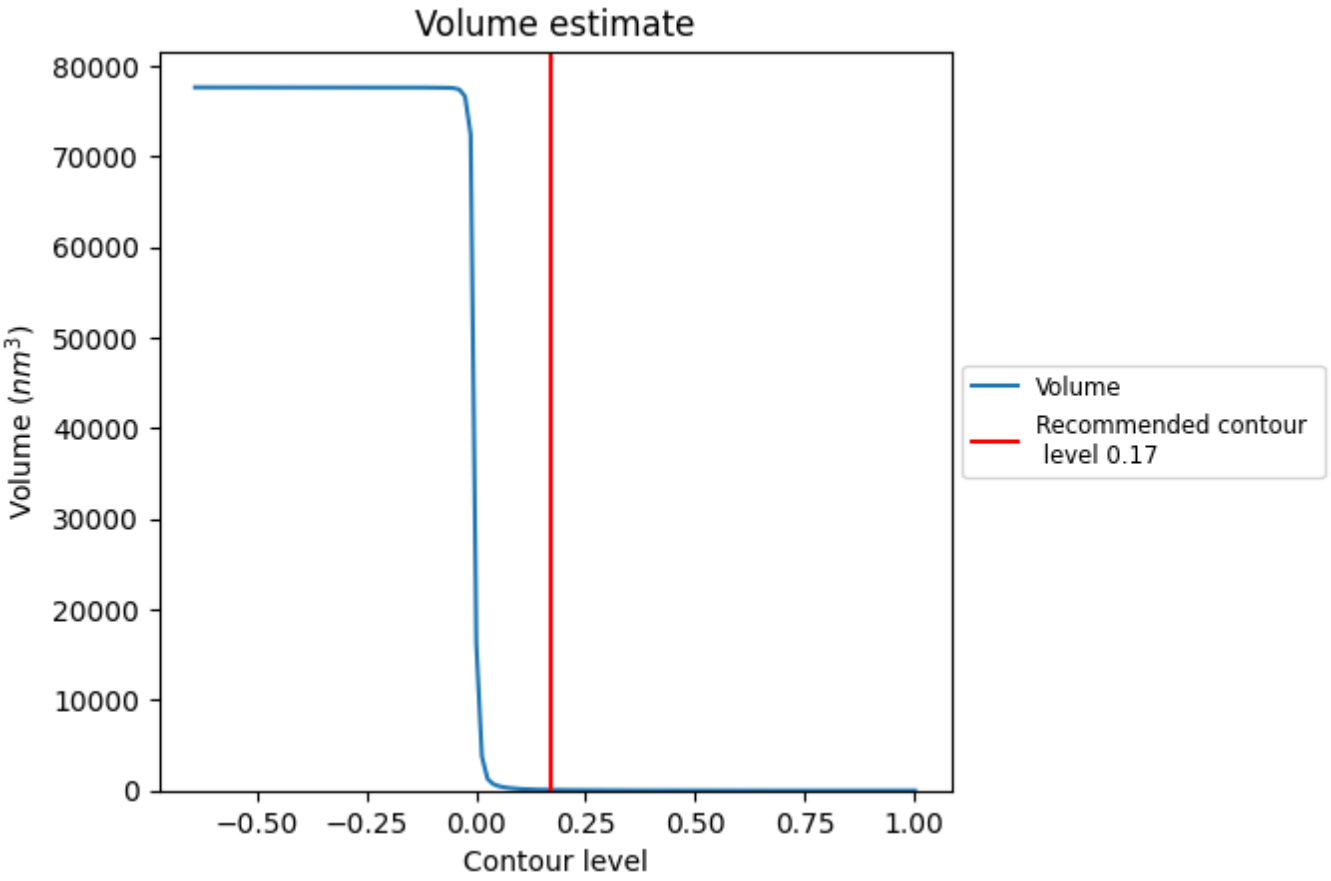
This section contains the results of statistical analysis of the map.

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.

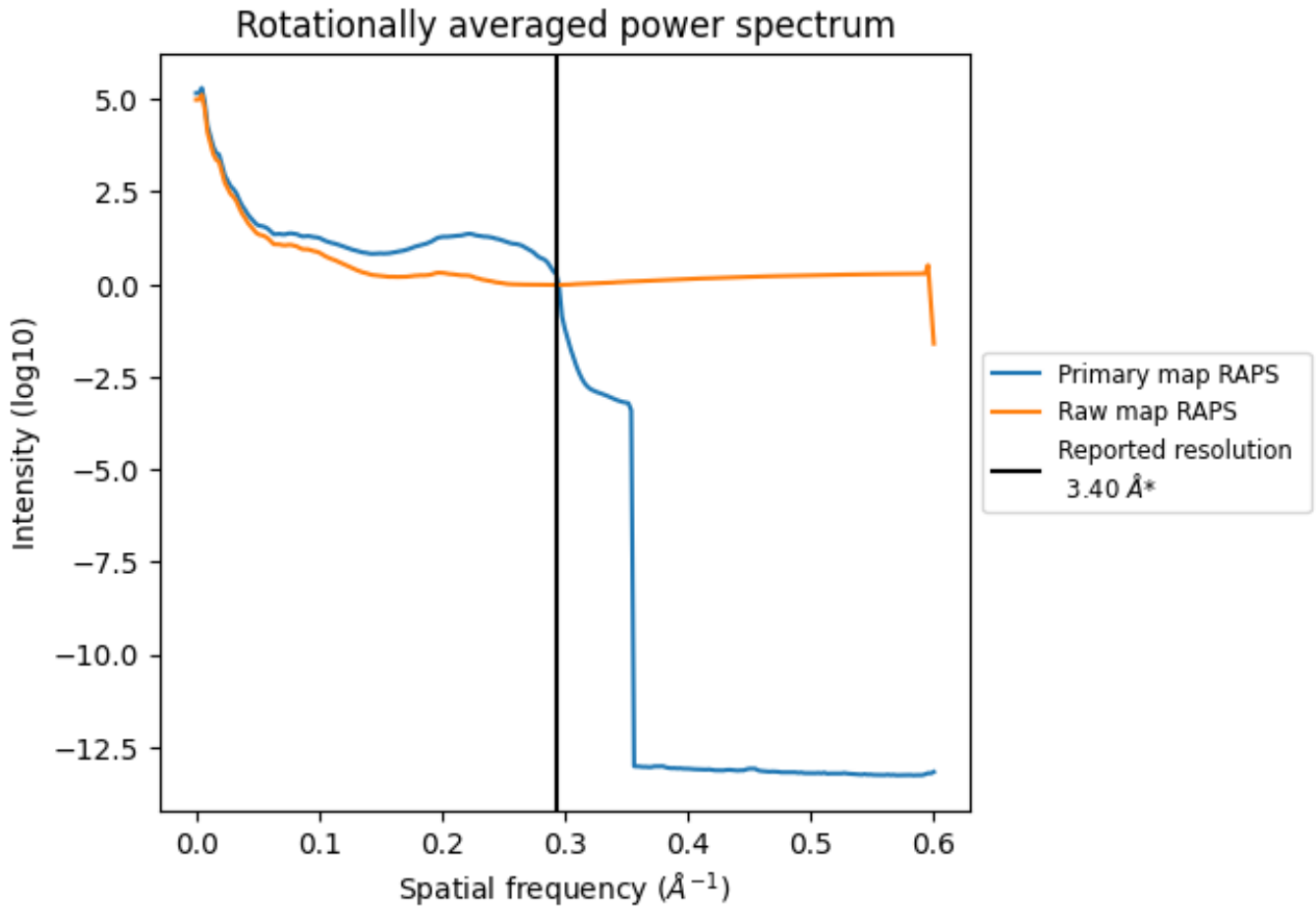
7.2 Volume estimate (i)



The volume at the recommended contour level is 77 nm^3; this corresponds to an approximate mass of 70 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)

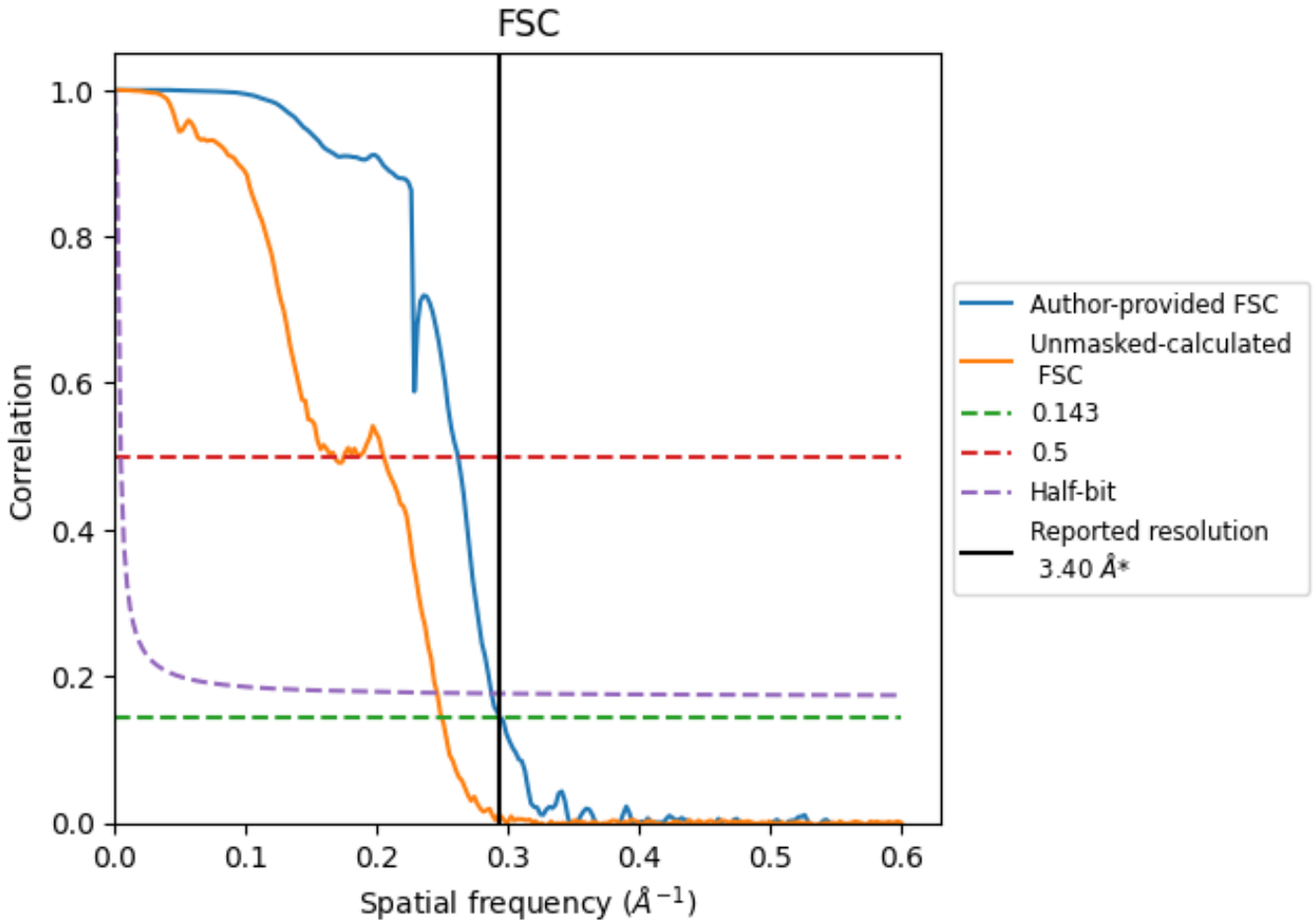


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

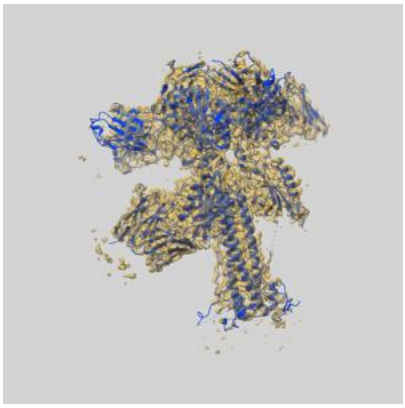
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.82	3.48
Unmasked-calculated*	4.01	5.97	4.07

*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 4.01 differs from the reported value 3.4 by more than 10 %

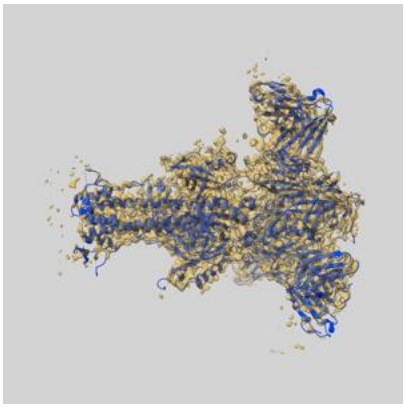
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43667 and PDB model 8VYM. Per-residue inclusion information can be found in section 3 on page 14.

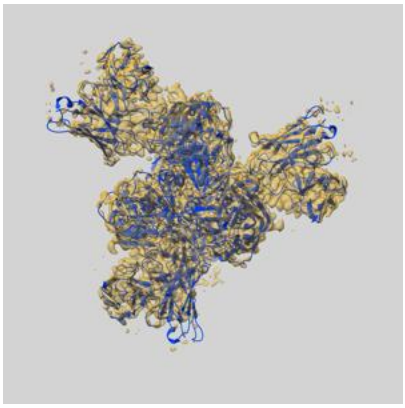
9.1 Map-model overlay



X



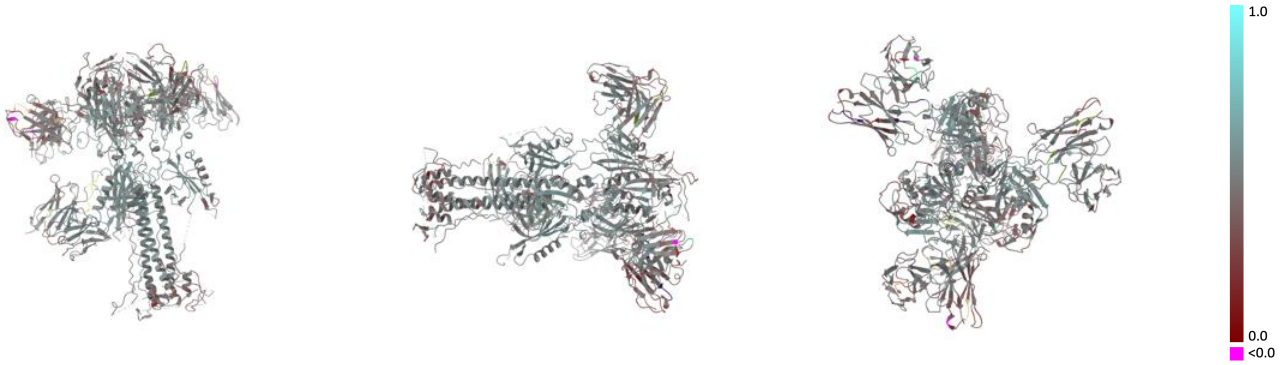
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 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.

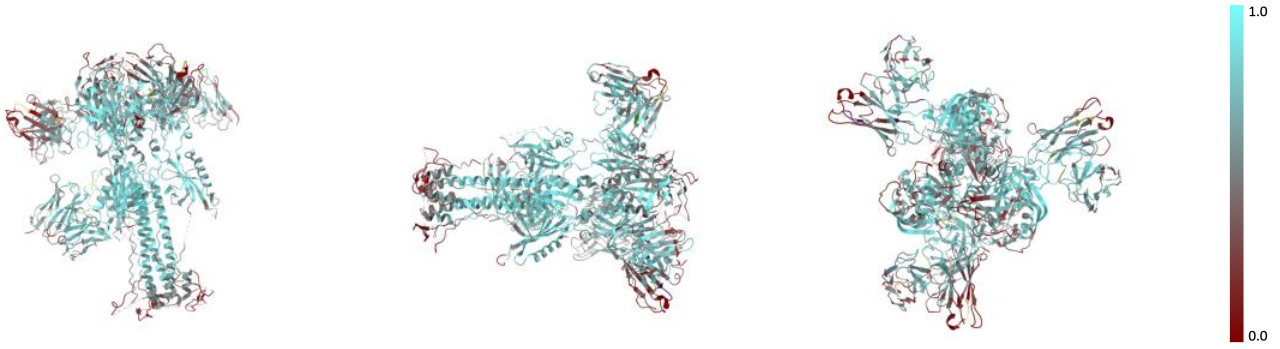
9.2 Q-score mapped to coordinate model (i)



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.

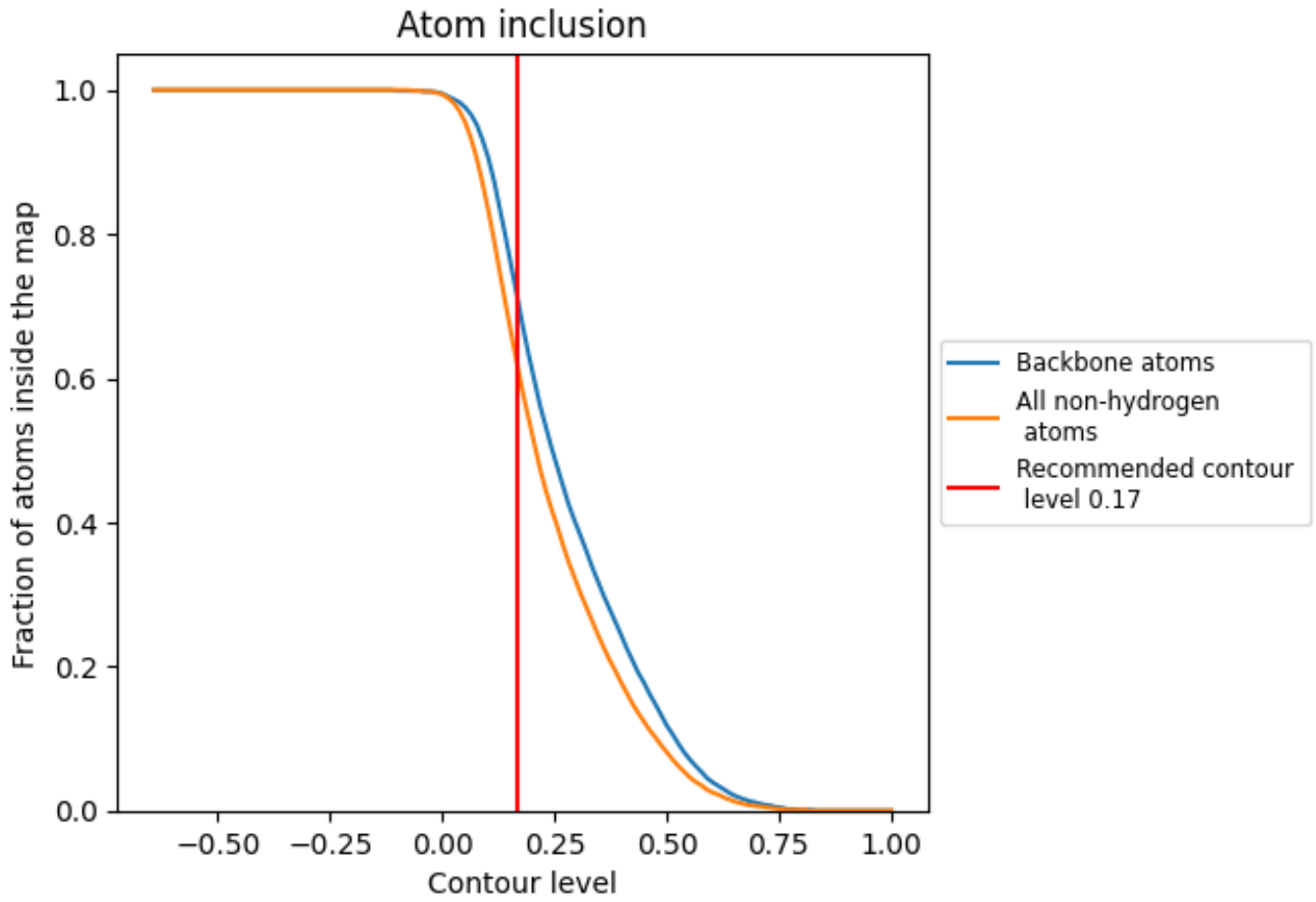
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 61% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6130	0.4760
A	0.6470	0.4970
B	0.6460	0.4920
C	0.6520	0.4920
D	0.4440	0.4240
E	0.5020	0.4420
F	0.6440	0.4640
G	0.5740	0.4550
H	0.6710	0.4810
I	0.5650	0.4510
J	0.5250	0.4310
K	0.6790	0.4910
L	0.6430	0.4620
M	0.2500	0.3890
N	0.3930	0.4110
O	0.1790	0.4480
P	0.5360	0.4250
Q	0.6790	0.5060
R	0.4870	0.4360
S	0.2140	0.3140
T	0.1790	0.2950
U	0.4290	0.3920
V	0.6150	0.5110
W	0.5130	0.4830
X	0.1790	0.4320
Y	0.2500	0.3440
Z	0.3930	0.3620
a	0.0360	0.2850