



## Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 09:18 AM EDT

PDB ID : 8VYN / pdb\_00008vyn  
EMDB ID : EMD-43672  
Title : Soluble ectodomain of human cytomegalovirus (HCMV) glycoprotein B (gB) stabilized in a prefusion-like conformation in complex with 1G2 and 7H3, composite map (global and local) and model  
Authors : Sponholtz, M.R.; Byrne, P.O.; McLellan, J.S.  
Deposited on : 2024-02-09  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1



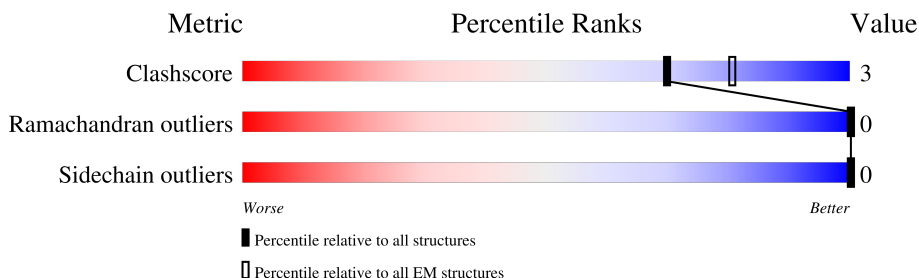
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	786	
1	C	786	
2	D	234	
2	H	234	
2	L	234	
3	E	216	
3	I	216	

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Mol	Chain	Length	Quality of chain
3	M	216	<div> <div>9%</div> <div>45%</div> <div>5%</div> <div>50%</div> </div>
4	F	224	<div> <div>12%</div> <div>44%</div> <div>9%</div> <div>47%</div> </div>
4	J	224	<div> <div>12%</div> <div>43%</div> <div>9%</div> <div>47%</div> </div>
4	N	224	<div> <div>12%</div> <div>43%</div> <div>9%</div> <div>47%</div> </div>
5	G	214	<div> <div>13%</div> <div>44%</div> <div>6%</div> <div>50%</div> </div>
5	K	214	<div> <div>13%</div> <div>44%</div> <div>6%</div> <div>50%</div> </div>
5	O	214	<div> <div>13%</div> <div>44%</div> <div>6%</div> <div>50%</div> </div>
6	P	3	<div> <div>33%</div> <div>100%</div> </div>
6	S	3	<div> <div>33%</div> <div>100%</div> </div>
6	V	3	<div> <div>33%</div> <div>100%</div> </div>
7	Q	2	<div> <div>50%</div> <div>100%</div> </div>
7	R	2	<div> <div>50%</div> <div>100%</div> </div>
7	T	2	<div> <div>50%</div> <div>100%</div> </div>
7	U	2	<div> <div>50%</div> <div>100%</div> </div>
7	W	2	<div> <div>50%</div> <div>100%</div> </div>
7	X	2	<div> <div>50%</div> <div>100%</div> </div>



## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23763 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	523	Total	C	N	O	S	0	0
			4206	2660	709	810	27		
1	B	523	Total	C	N	O	S	0	0
			4206	2660	709	810	27		
1	C	523	Total	C	N	O	S	0	0
			4206	2660	709	810	27		

There are 273 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	LEU	THR	engineered mutation	UNP P13201
A	134	CYS	VAL	engineered mutation	UNP P13201
A	222	CYS	HIS	engineered mutation	UNP P13201
A	246	SER	CYS	conflict	UNP P13201
A	267	ILE	ALA	engineered mutation	UNP P13201
A	457	SER	ARG	conflict	UNP P13201
A	460	SER	ARG	conflict	UNP P13201
A	653	CYS	ILE	engineered mutation	UNP P13201
A	657	CYS	GLU	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	100	LEU	THR	engineered mutation	UNP P13201
B	134	CYS	VAL	engineered mutation	UNP P13201
B	222	CYS	HIS	engineered mutation	UNP P13201
B	246	SER	CYS	conflict	UNP P13201
B	267	ILE	ALA	engineered mutation	UNP P13201
B	457	SER	ARG	conflict	UNP P13201
B	460	SER	ARG	conflict	UNP P13201
B	653	CYS	ILE	engineered mutation	UNP P13201
B	657	CYS	GLU	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	100	LEU	THR	engineered mutation	UNP P13201
C	134	CYS	VAL	engineered mutation	UNP P13201
C	222	CYS	HIS	engineered mutation	UNP P13201
C	246	SER	CYS	conflict	UNP P13201
C	267	ILE	ALA	engineered mutation	UNP P13201
C	457	SER	ARG	conflict	UNP P13201
C	460	SER	ARG	conflict	UNP P13201
C	653	CYS	ILE	engineered mutation	UNP P13201
C	657	CYS	GLU	engineered mutation	UNP P13201
C	705	GLY	-	expression tag	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 7H3 Fab Heavy Chain.



Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	130	Total	C	N	O	S	0	0
			1017	643	170	197	7		
2	H	130	Total	C	N	O	S	0	0
			1017	643	170	197	7		
2	L	130	Total	C	N	O	S	0	0
			1017	643	170	197	7		

- Molecule 3 is a protein called 7H3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	108	Total	C	N	O	S	0	0
			797	495	139	160	3		
3	I	108	Total	C	N	O	S	0	0
			797	495	139	160	3		
3	M	108	Total	C	N	O	S	0	0
			797	495	139	160	3		

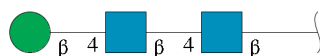
- Molecule 4 is a protein called 1G2 Fab Heavy Chain.

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

- Molecule 5 is a protein called 1G2 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	107	Total	C	N	O	S	0	0
			806	499	139	166	2		
5	K	107	Total	C	N	O	S	0	0
			806	499	139	166	2		
5	O	107	Total	C	N	O	S	0	0
			806	499	139	166	2		

- Molecule 6 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
6	P	3	Total	C	N	O	0	0
			39	22	2	15		
6	S	3	Total	C	N	O	0	0
			39	22	2	15		
6	V	3	Total	C	N	O	0	0
			39	22	2	15		

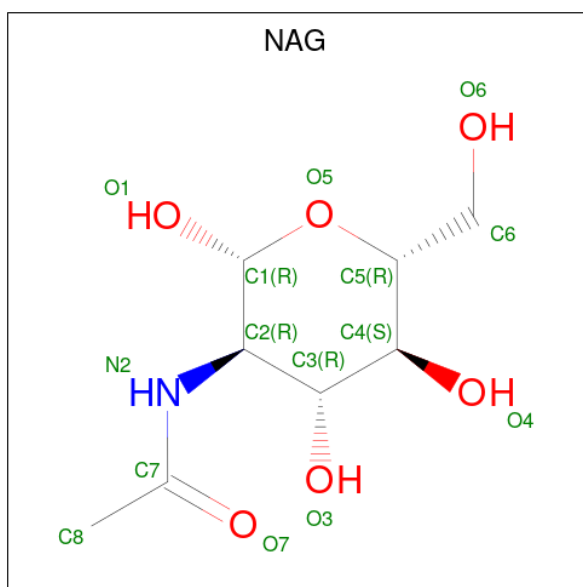
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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





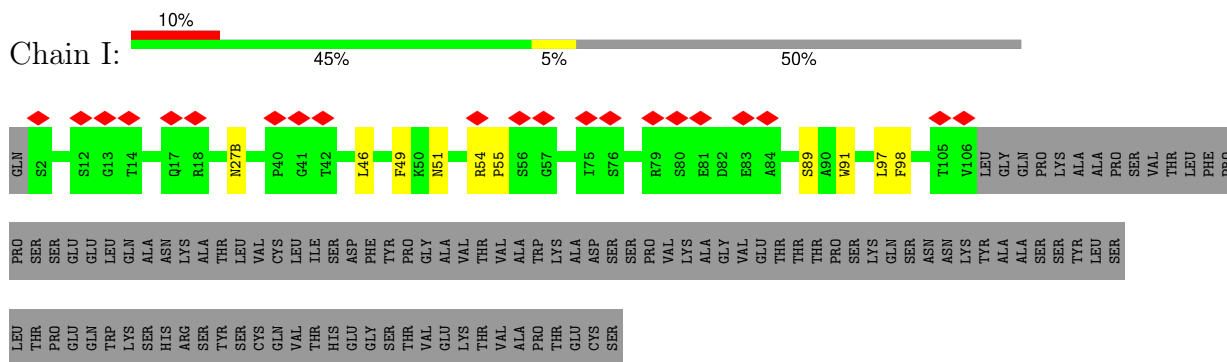




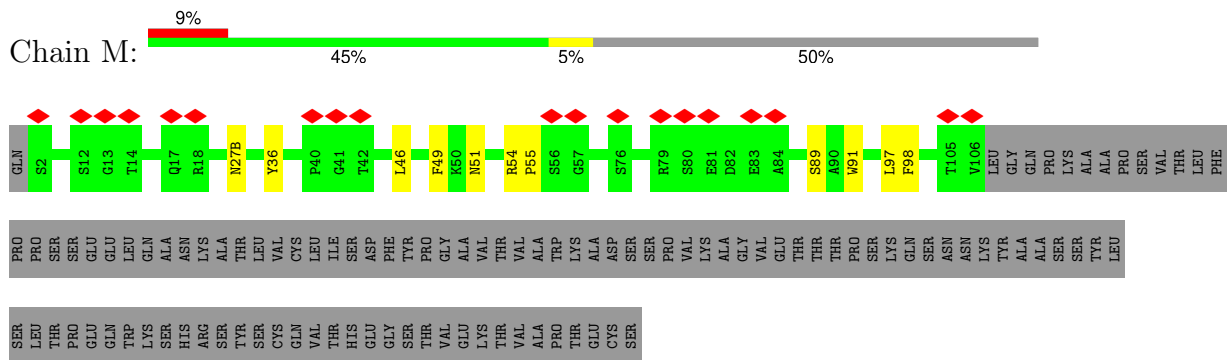




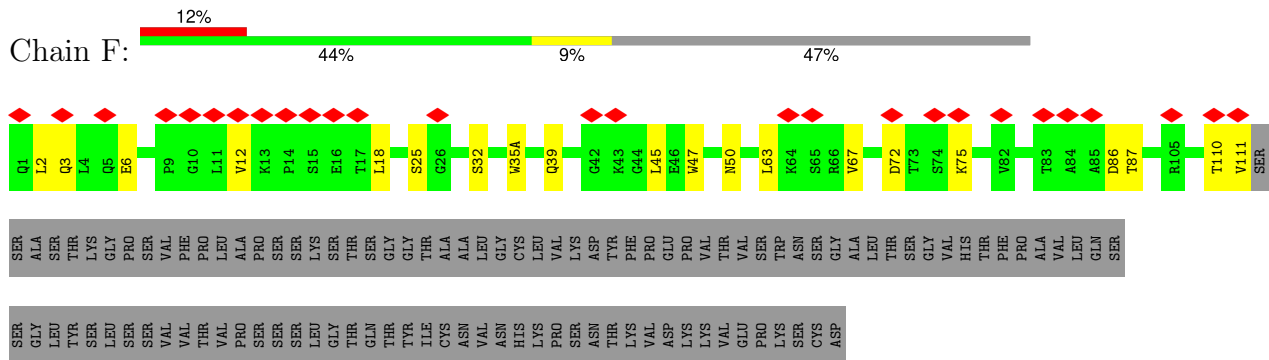




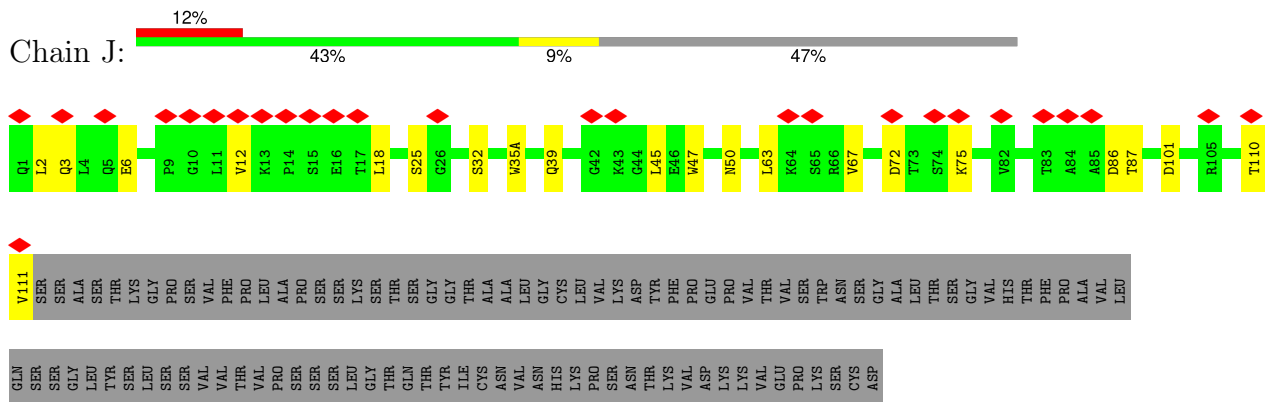
- Molecule 3: 7H3 Fab Light Chain



- Molecule 4: 1G2 Fab Heavy Chain



- Molecule 4: 1G2 Fab Heavy Chain



- Molecule 4: 1G2 Fab Heavy Chain







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

Chain P: 



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

Chain S: 



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

Chain V: 



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

Chain Q: 



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

Chain R: 



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

Chain T: 





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



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



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	165982	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 ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.885	Depositor
Minimum map value	-1.400	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	399.93597, 399.93597, 399.93597	wwPDB
Map dimensions	480, 480, 480	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: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.17	0/4293	0.34	0/5816
1	B	0.17	0/4293	0.34	0/5816
1	C	0.17	0/4293	0.34	0/5816
2	D	0.15	0/1044	0.29	0/1417
2	H	0.15	0/1044	0.29	0/1417
2	L	0.15	0/1044	0.30	0/1417
3	E	0.14	0/816	0.35	0/1107
3	I	0.14	0/816	0.35	0/1107
3	M	0.14	0/816	0.34	0/1107
4	F	0.16	0/971	0.33	0/1325
4	J	0.16	0/971	0.33	0/1325
4	N	0.16	0/971	0.33	0/1325
5	G	0.15	0/826	0.37	0/1125
5	K	0.15	0/826	0.37	0/1125
5	O	0.15	0/826	0.37	0/1125
All	All	0.16	0/23850	0.34	0/32370

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.

There are no bond angle outliers.



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Sidechain
1	B	320	ARG	Sidechain
1	C	320	ARG	Sidechain

## 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	4206	0	4056	23	0
1	B	4206	0	4056	26	0
1	C	4206	0	4056	25	0
2	D	1017	0	953	9	0
2	H	1017	0	953	9	0
2	L	1017	0	953	10	0
3	E	797	0	770	5	0
3	I	797	0	770	6	0
3	M	797	0	770	7	0
4	F	944	0	920	11	0
4	J	944	0	920	12	0
4	N	944	0	920	12	0
5	G	806	0	761	7	0
5	K	806	0	761	6	0
5	O	806	0	761	7	0
6	P	39	0	34	0	0
6	S	39	0	34	0	0
6	V	39	0	34	0	0
7	Q	28	0	25	0	0
7	R	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
8	A	56	0	52	0	0
8	B	56	0	52	0	0
8	C	56	0	52	0	0
All	All	23763	0	22788	156	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.

All (156) 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:127:VAL:HG22	1:C:430:PHE:HB2	1.71	0.73
1:A:127:VAL:HG22	1:A:430:PHE:HB2	1.72	0.71
5:O:2:SER:OG	5:O:27(B):ASN:ND2	2.24	0.71
1:B:127:VAL:HG22	1:B:430:PHE:HB2	1.73	0.70
1:A:323:ALA:HB2	1:A:336:ILE:HD11	1.74	0.69
1:C:323:ALA:HB2	1:C:336:ILE:HD11	1.75	0.69
5:K:2:SER:OG	5:K:27(B):ASN:ND2	2.24	0.69
5:G:2:SER:OG	5:G:27(B):ASN:ND2	2.25	0.69
1:A:649:ILE:HG21	1:B:130:LYS:HD2	1.76	0.68
1:A:118:ASN:ND2	1:A:120:ASP:OD1	2.27	0.68
1:B:323:ALA:HB2	1:B:336:ILE:HD11	1.76	0.67
2:D:18:VAL:HG23	2:D:82(C):LEU:HD11	1.77	0.67
2:L:18:VAL:HG23	2:L:82(C):LEU:HD11	1.77	0.67
2:H:18:VAL:HG23	2:H:82(C):LEU:HD11	1.77	0.67
1:B:118:ASN:ND2	1:B:120:ASP:OD1	2.27	0.66
1:B:649:ILE:HG21	1:C:130:LYS:HD2	1.78	0.66
1:A:408:TYR:HB3	1:A:412:TYR:HB2	1.79	0.65
1:A:130:LYS:HD2	1:C:649:ILE:HG21	1.77	0.65
1:B:408:TYR:HB3	1:B:412:TYR:HB2	1.79	0.64
1:C:408:TYR:HB3	1:C:412:TYR:HB2	1.80	0.63
1:C:118:ASN:ND2	1:C:120:ASP:OD1	2.29	0.63
4:J:39:GLN:HB2	4:J:45:LEU:HD23	1.82	0.62
4:F:39:GLN:HB2	4:F:45:LEU:HD23	1.83	0.61
4:N:39:GLN:HB2	4:N:45:LEU:HD23	1.82	0.61
4:F:72:ASP:OD2	4:F:75:LYS:NZ	2.28	0.59
1:C:342:VAL:HG13	1:C:343:THR:HG23	1.85	0.58
4:J:72:ASP:OD2	4:J:75:LYS:NZ	2.28	0.58
4:J:87:THR:HG23	4:J:110:THR:HA	1.86	0.58
4:N:87:THR:HG23	4:N:110:THR:HA	1.86	0.57
4:F:87:THR:HG23	4:F:110:THR:HA	1.86	0.57
1:A:342:VAL:HG13	1:A:343:THR:HG23	1.86	0.57
4:N:72:ASP:OD2	4:N:75:LYS:NZ	2.27	0.57
1:B:342:VAL:HG13	1:B:343:THR:HG23	1.86	0.56
2:D:87:THR:HA	2:D:109:VAL:O	2.06	0.56
2:L:35:HIS:NE2	2:L:95:ASP:OD2	2.28	0.56
2:L:87:THR:HA	2:L:109:VAL:O	2.06	0.56
2:H:87:THR:HA	2:H:109:VAL:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:88:CYS:O	5:K:99:GLY:N	2.39	0.56
5:O:88:CYS:O	5:O:99:GLY:N	2.39	0.55
5:G:88:CYS:O	5:G:99:GLY:N	2.39	0.55
1:A:304:THR:HG21	1:A:316:LEU:HD12	1.90	0.54
2:D:35:HIS:NE2	2:D:95:ASP:OD2	2.29	0.54
1:B:304:THR:HG21	1:B:316:LEU:HD12	1.91	0.53
2:H:35:HIS:NE2	2:H:95:ASP:OD2	2.30	0.53
1:C:304:THR:HG21	1:C:316:LEU:HD12	1.90	0.53
4:F:6:GLU:N	4:F:6:GLU:OE1	2.42	0.53
1:A:294:ALA:HB2	4:F:32:SER:HA	1.90	0.52
4:N:6:GLU:OE1	4:N:6:GLU:N	2.42	0.52
1:B:294:ALA:HB2	4:J:32:SER:HA	1.91	0.52
3:I:89:SER:HA	3:I:97:LEU:O	2.10	0.52
3:E:46:LEU:HD21	3:E:49:PHE:HB3	1.92	0.52
1:C:294:ALA:HB2	4:N:32:SER:HA	1.91	0.51
4:J:6:GLU:OE1	4:J:6:GLU:N	2.43	0.51
2:L:83:ARG:N	2:L:86:ASP:OD2	2.41	0.51
1:A:124:GLY:HA2	1:A:434:ILE:HG12	1.93	0.51
1:A:259:SER:HB3	1:A:266:PHE:HB3	1.92	0.51
3:E:89:SER:HA	3:E:97:LEU:O	2.12	0.50
1:C:124:GLY:HA2	1:C:434:ILE:HG12	1.93	0.50
3:I:27(B):ASN:HA	3:I:91:TRP:O	2.12	0.50
3:I:46:LEU:HD21	3:I:49:PHE:HB3	1.94	0.50
4:N:3:GLN:HB2	4:N:25:SER:HB3	1.94	0.50
5:G:32:TYR:HA	5:G:51:ASN:HD21	1.77	0.50
3:M:89:SER:HA	3:M:97:LEU:O	2.11	0.50
1:B:124:GLY:HA2	1:B:434:ILE:HG12	1.93	0.49
5:K:92:ASP:OD1	5:K:93:ASP:N	2.42	0.49
5:O:4:LEU:HD11	5:O:90:THR:HG22	1.95	0.49
5:O:32:TYR:HA	5:O:51:ASN:HD21	1.78	0.49
5:K:5:THR:HB	5:K:24:SER:HB2	1.95	0.49
1:C:423:THR:HG22	1:C:425:GLY:H	1.77	0.49
1:B:423:THR:HG22	1:B:425:GLY:H	1.78	0.49
1:A:423:THR:HG22	1:A:425:GLY:H	1.77	0.49
1:C:259:SER:HB3	1:C:266:PHE:HB3	1.94	0.49
3:M:27(B):ASN:HA	3:M:91:TRP:O	2.13	0.49
5:K:32:TYR:HA	5:K:51:ASN:HD21	1.77	0.49
1:B:259:SER:HB3	1:B:266:PHE:HB3	1.94	0.48
4:F:3:GLN:HB2	4:F:25:SER:HB3	1.94	0.48
5:O:92:ASP:OD1	5:O:93:ASP:N	2.41	0.48
4:J:3:GLN:HB2	4:J:25:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:4:LEU:HD11	5:K:90:THR:HG22	1.94	0.48
4:F:47:TRP:HE1	4:F:50:ASN:ND2	2.12	0.48
3:M:46:LEU:HD21	3:M:49:PHE:HB3	1.95	0.48
3:E:27(B):ASN:HA	3:E:91:TRP:O	2.13	0.48
4:J:47:TRP:HE1	4:J:50:ASN:ND2	2.11	0.48
4:N:47:TRP:HE1	4:N:50:ASN:ND2	2.12	0.47
5:G:4:LEU:HD11	5:G:90:THR:HG22	1.95	0.47
5:G:5:THR:HB	5:G:24:SER:HB2	1.96	0.47
5:O:5:THR:HB	5:O:24:SER:HB2	1.95	0.47
4:N:12:VAL:HG21	4:N:18:LEU:HD13	1.97	0.47
4:N:101:ASP:OD1	4:N:101:ASP:N	2.42	0.47
1:B:399:LYS:HB2	1:B:399:LYS:HE2	1.73	0.46
2:D:17:SER:HA	2:D:82:LEU:O	2.16	0.46
2:D:83:ARG:N	2:D:86:ASP:OD2	2.43	0.46
4:J:12:VAL:HG21	4:J:18:LEU:HD13	1.98	0.46
1:C:361:GLU:CD	3:M:51:ASN:HD21	2.24	0.46
2:L:100(J):TYR:HH	3:M:36:TYR:HH	1.56	0.45
1:B:658:ASN:ND2	1:C:95:SER:HB3	2.31	0.45
1:C:399:LYS:HB2	1:C:399:LYS:HE2	1.73	0.45
2:D:38:ARG:O	2:D:46:GLU:N	2.40	0.45
4:J:2:LEU:HD11	4:J:35(A):TRP:HH2	1.81	0.45
4:J:101:ASP:OD1	4:J:101:ASP:N	2.42	0.45
1:B:381:GLU:HG2	1:B:421:PHE:CE1	2.52	0.45
2:H:83:ARG:N	2:H:86:ASP:OD2	2.42	0.45
2:L:17:SER:HA	2:L:82:LEU:O	2.16	0.45
4:F:12:VAL:HG21	4:F:18:LEU:HD13	1.99	0.44
5:G:92:ASP:OD1	5:G:93:ASP:N	2.42	0.44
2:H:17:SER:HA	2:H:82:LEU:O	2.17	0.44
1:A:381:GLU:HG2	1:A:421:PHE:CE1	2.52	0.44
1:B:361:GLU:CD	3:I:51:ASN:HD21	2.26	0.44
1:C:301:PRO:HA	1:C:321:LEU:HD23	2.00	0.44
1:C:381:GLU:HG2	1:C:421:PHE:CE1	2.52	0.44
1:A:95:SER:HB3	1:C:658:ASN:ND2	2.32	0.44
1:A:361:GLU:CD	3:E:51:ASN:HD21	2.26	0.44
1:A:491:LEU:HD21	1:C:491:LEU:HB3	2.00	0.44
4:N:2:LEU:HD11	4:N:35(A):TRP:HH2	1.83	0.44
1:B:491:LEU:HB3	1:C:491:LEU:HD21	2.00	0.44
2:D:35:HIS:CD2	2:D:95:ASP:HB2	2.53	0.44
2:H:35:HIS:CD2	2:H:95:ASP:HB2	2.52	0.43
4:N:86:ASP:HB2	4:N:111:VAL:HG21	2.00	0.43
4:J:86:ASP:HB2	4:J:111:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2:LEU:HD11	4:F:35(A):TRP:HH2	1.83	0.43
2:L:35:HIS:CD2	2:L:95:ASP:HB2	2.53	0.43
1:A:126:MET:HE1	1:A:375:PHE:CD2	2.54	0.43
1:A:658:ASN:ND2	1:B:95:SER:HB3	2.33	0.43
1:B:301:PRO:HA	1:B:321:LEU:HD23	2.00	0.43
1:A:301:PRO:HA	1:A:321:LEU:HD23	2.01	0.43
1:A:491:LEU:HB3	1:B:491:LEU:HD21	2.00	0.43
1:B:506:TRP:O	1:B:510:GLN:HG2	2.19	0.43
2:H:100(M):MET:HE1	3:I:98:PHE:CZ	2.53	0.43
1:A:506:TRP:O	1:A:510:GLN:HG2	2.19	0.42
1:B:126:MET:HE1	1:B:375:PHE:CD2	2.55	0.42
1:C:126:MET:HE1	1:C:375:PHE:CD2	2.54	0.42
4:F:86:ASP:HB2	4:F:111:VAL:HG21	2.01	0.42
2:D:12:LYS:HG3	2:D:18:VAL:HG22	2.02	0.42
4:N:63:LEU:O	4:N:67:VAL:HB	2.20	0.42
4:F:63:LEU:O	4:F:67:VAL:HB	2.20	0.42
2:L:100(M):MET:HE1	3:M:98:PHE:CZ	2.55	0.42
1:C:506:TRP:O	1:C:510:GLN:HG2	2.19	0.41
4:J:63:LEU:O	4:J:67:VAL:HB	2.20	0.41
1:B:127:VAL:CG2	1:B:430:PHE:HB2	2.48	0.41
1:C:80:ASP:HB3	1:C:560:LYS:HB3	2.02	0.41
2:H:52(A):PRO:O	2:H:71:ARG:NH1	2.54	0.41
3:M:54:ARG:HA	3:M:55:PRO:HD3	1.94	0.41
1:B:488:TYR:OH	1:B:492:ARG:NH1	2.53	0.41
1:B:80:ASP:HB3	1:B:560:LYS:HB3	2.01	0.41
1:B:365:HIS:NE2	1:B:504:GLU:OE2	2.54	0.41
1:C:488:TYR:OH	1:C:492:ARG:NH1	2.54	0.41
2:H:70:THR:OG1	2:H:79:TYR:HB2	2.21	0.41
5:O:33:VAL:H	5:O:51:ASN:ND2	2.18	0.41
2:D:100(J):TYR:HB3	3:E:91:TRP:HB2	2.03	0.41
1:C:365:HIS:NE2	1:C:504:GLU:OE2	2.54	0.40
1:A:127:VAL:CG2	1:A:430:PHE:HB2	2.47	0.40
3:I:54:ARG:HA	3:I:55:PRO:HD3	1.94	0.40
2:L:6:GLN:HE21	2:L:20:VAL:HG11	1.86	0.40
1:A:365:HIS:NE2	1:A:504:GLU:OE2	2.52	0.40
2:L:12:LYS:HG3	2:L:18:VAL:HG22	2.02	0.40
5:G:33:VAL:H	5:G:51:ASN:ND2	2.19	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	513/786 (65%)	486 (95%)	27 (5%)	0	100	100
1	B	513/786 (65%)	486 (95%)	27 (5%)	0	100	100
1	C	513/786 (65%)	486 (95%)	27 (5%)	0	100	100
2	D	128/234 (55%)	125 (98%)	3 (2%)	0	100	100
2	H	128/234 (55%)	125 (98%)	3 (2%)	0	100	100
2	L	128/234 (55%)	125 (98%)	3 (2%)	0	100	100
3	E	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
3	I	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
3	M	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
4	F	116/224 (52%)	111 (96%)	5 (4%)	0	100	100
4	J	116/224 (52%)	111 (96%)	5 (4%)	0	100	100
4	N	116/224 (52%)	111 (96%)	5 (4%)	0	100	100
5	G	105/214 (49%)	97 (92%)	8 (8%)	0	100	100
5	K	105/214 (49%)	97 (92%)	8 (8%)	0	100	100
5	O	105/214 (49%)	97 (92%)	8 (8%)	0	100	100
All	All	2904/5022 (58%)	2760 (95%)	144 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	472/696 (68%)	472 (100%)	0	100	100
1	B	472/696 (68%)	472 (100%)	0	100	100
1	C	472/696 (68%)	472 (100%)	0	100	100
2	D	107/197 (54%)	107 (100%)	0	100	100
2	H	107/197 (54%)	107 (100%)	0	100	100
2	L	107/197 (54%)	107 (100%)	0	100	100
3	E	89/182 (49%)	89 (100%)	0	100	100
3	I	89/182 (49%)	89 (100%)	0	100	100
3	M	89/182 (49%)	89 (100%)	0	100	100
4	F	102/194 (53%)	102 (100%)	0	100	100
4	J	102/194 (53%)	102 (100%)	0	100	100
4	N	102/194 (53%)	102 (100%)	0	100	100
5	G	90/182 (50%)	90 (100%)	0	100	100
5	K	90/182 (50%)	90 (100%)	0	100	100
5	O	90/182 (50%)	90 (100%)	0	100	100
All	All	2580/4353 (59%)	2580 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	220	ASN
1	A	341	ASN
1	A	345	GLN
1	A	447	ASN
1	A	478	ASN
1	A	483	GLN
1	A	556	GLN
1	A	566	ASN
1	B	85	ASN
1	B	202	HIS
1	B	220	ASN
1	B	341	ASN
1	B	345	GLN
1	B	447	ASN

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Mol	Chain	Res	Type
1	B	478	ASN
1	B	483	GLN
1	B	556	GLN
1	C	85	ASN
1	C	202	HIS
1	C	220	ASN
1	C	341	ASN
1	C	345	GLN
1	C	447	ASN
1	C	478	ASN
1	C	556	GLN
1	C	566	ASN
1	C	583	ASN
2	D	39	GLN
3	E	38	GLN
3	E	51	ASN
4	F	50	ASN
4	F	76	ASN
4	F	77	GLN
5	G	17	GLN
5	G	51	ASN
3	I	51	ASN
4	J	50	ASN
4	J	76	ASN
4	J	77	GLN
5	K	17	GLN
5	K	51	ASN
2	L	39	GLN
3	M	38	GLN
3	M	51	ASN
4	N	50	ASN
4	N	76	ASN
4	N	77	GLN
5	O	17	GLN
5	O	51	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

21 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	P	1	6,1	14,14,15	0.76	0	17,19,21	0.99	1 (5%)
6	NAG	P	2	6	14,14,15	0.74	0	17,19,21	1.10	2 (11%)
6	BMA	P	3	6	11,11,12	0.80	0	15,15,17	1.13	1 (6%)
7	NAG	Q	1	7,1	14,14,15	0.77	0	17,19,21	0.98	1 (5%)
7	NAG	Q	2	7	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
7	NAG	R	1	7,1	14,14,15	0.73	0	17,19,21	0.80	0
7	NAG	R	2	7	14,14,15	0.70	0	17,19,21	0.87	0
6	NAG	S	1	6,1	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
6	NAG	S	2	6	14,14,15	0.74	0	17,19,21	1.09	2 (11%)
6	BMA	S	3	6	11,11,12	0.82	0	15,15,17	1.14	1 (6%)
7	NAG	T	1	7,1	14,14,15	0.78	0	17,19,21	0.98	1 (5%)
7	NAG	T	2	7	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
7	NAG	U	1	7,1	14,14,15	0.73	0	17,19,21	0.78	0
7	NAG	U	2	7	14,14,15	0.69	0	17,19,21	0.87	0
6	NAG	V	1	6,1	14,14,15	0.77	0	17,19,21	1.00	1 (5%)
6	NAG	V	2	6	14,14,15	0.75	0	17,19,21	1.08	2 (11%)
6	BMA	V	3	6	11,11,12	0.79	0	15,15,17	1.12	1 (6%)
7	NAG	W	1	7,1	14,14,15	0.79	0	17,19,21	0.97	1 (5%)
7	NAG	W	2	7	14,14,15	0.73	0	17,19,21	0.82	1 (5%)
7	NAG	X	1	7,1	14,14,15	0.73	0	17,19,21	0.77	0
7	NAG	X	2	7	14,14,15	0.70	0	17,19,21	0.89	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	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	NAG	R	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	BMA	S	3	6	-	0/2/19/22	0/1/1/1
7	NAG	T	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	NAG	U	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
7	NAG	W	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	3	BMA	C1-O5-C5	3.31	116.62	112.19
6	P	3	BMA	C1-O5-C5	3.23	116.51	112.19
6	V	3	BMA	C1-O5-C5	3.22	116.51	112.19
6	V	1	NAG	C1-O5-C5	2.96	116.15	112.19
6	P	1	NAG	C1-O5-C5	2.89	116.05	112.19
6	S	1	NAG	C1-O5-C5	2.85	116.01	112.19
6	V	2	NAG	C1-O5-C5	2.61	115.68	112.19
6	P	2	NAG	C1-O5-C5	2.59	115.65	112.19
6	S	2	NAG	C2-N2-C7	2.57	126.34	122.90
6	P	2	NAG	C2-N2-C7	2.54	126.31	122.90
6	S	2	NAG	C1-O5-C5	2.53	115.58	112.19
6	V	2	NAG	C2-N2-C7	2.41	126.13	122.90
7	Q	2	NAG	C1-O5-C5	2.25	115.21	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	2	NAG	C1-O5-C5	2.25	115.20	112.19
7	W	2	NAG	C1-O5-C5	2.21	115.15	112.19
7	W	1	NAG	C1-O5-C5	2.04	114.92	112.19
7	T	1	NAG	C1-O5-C5	2.02	114.90	112.19
7	Q	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

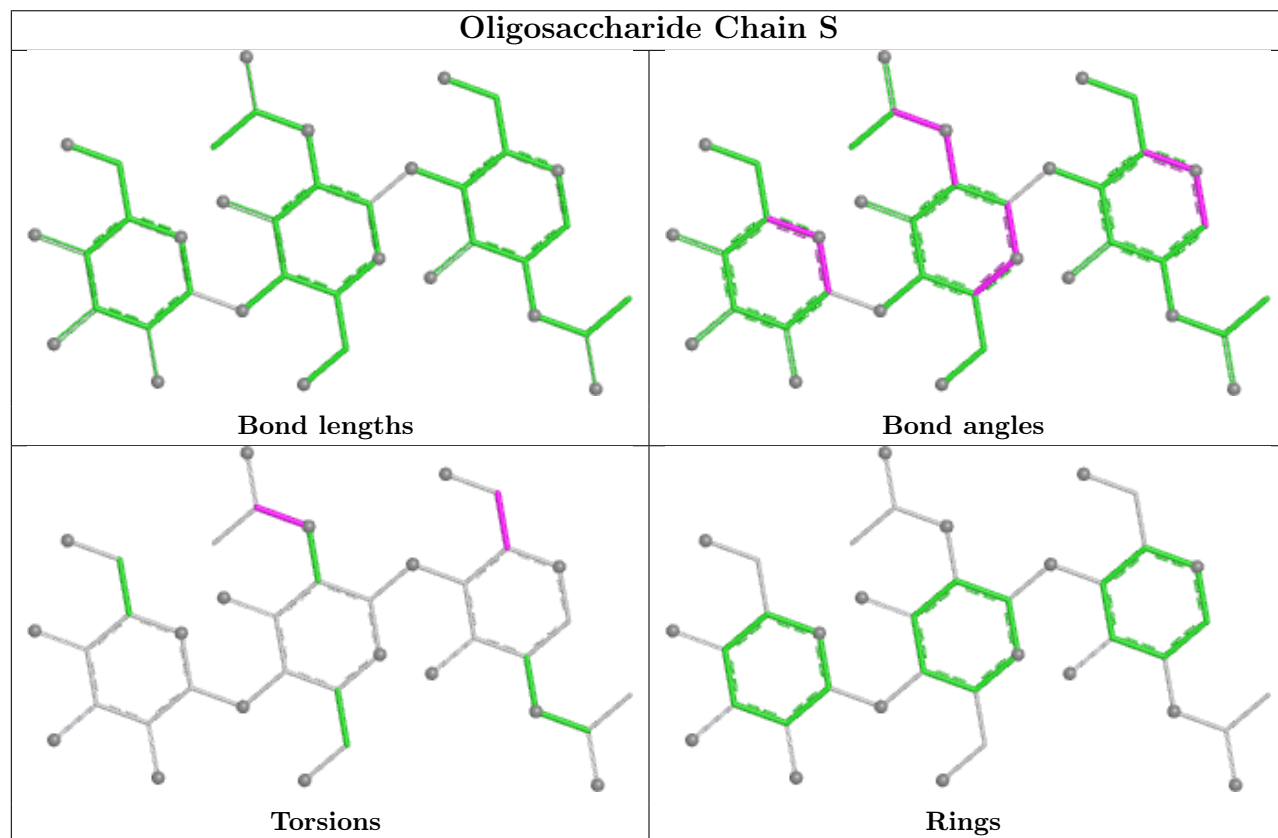
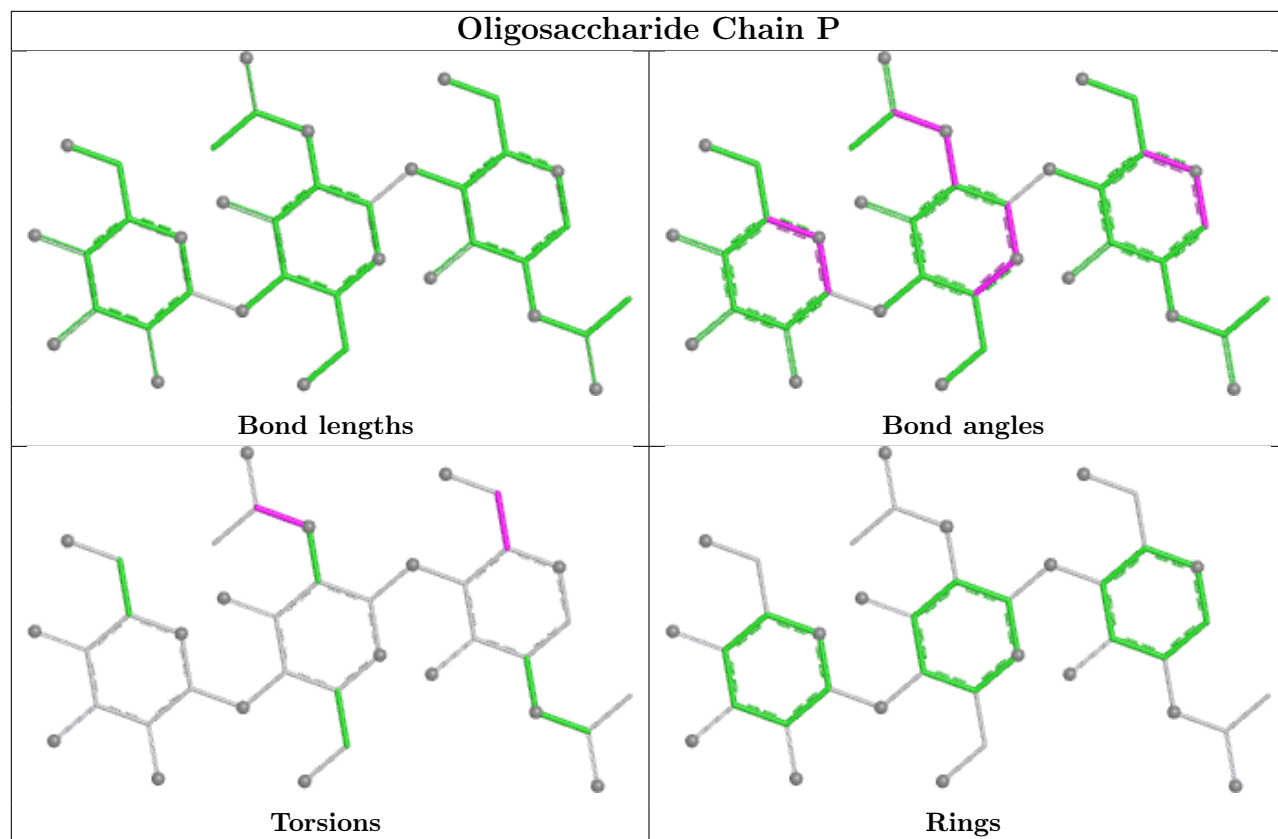
Mol	Chain	Res	Type	Atoms
6	P	1	NAG	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	P	2	NAG	C8-C7-N2-C2
6	P	2	NAG	O7-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
6	P	1	NAG	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6

There are no ring outliers.

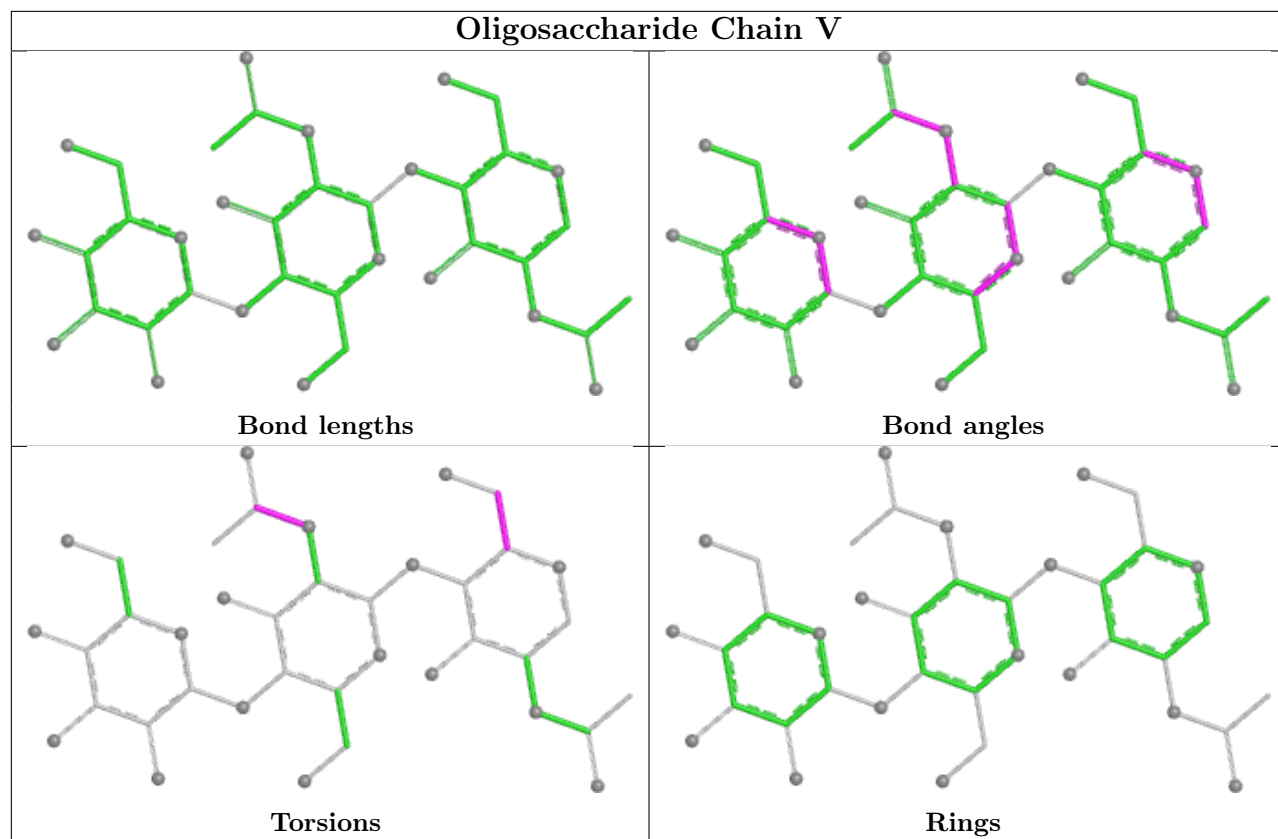
No monomer is involved in short contacts.

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

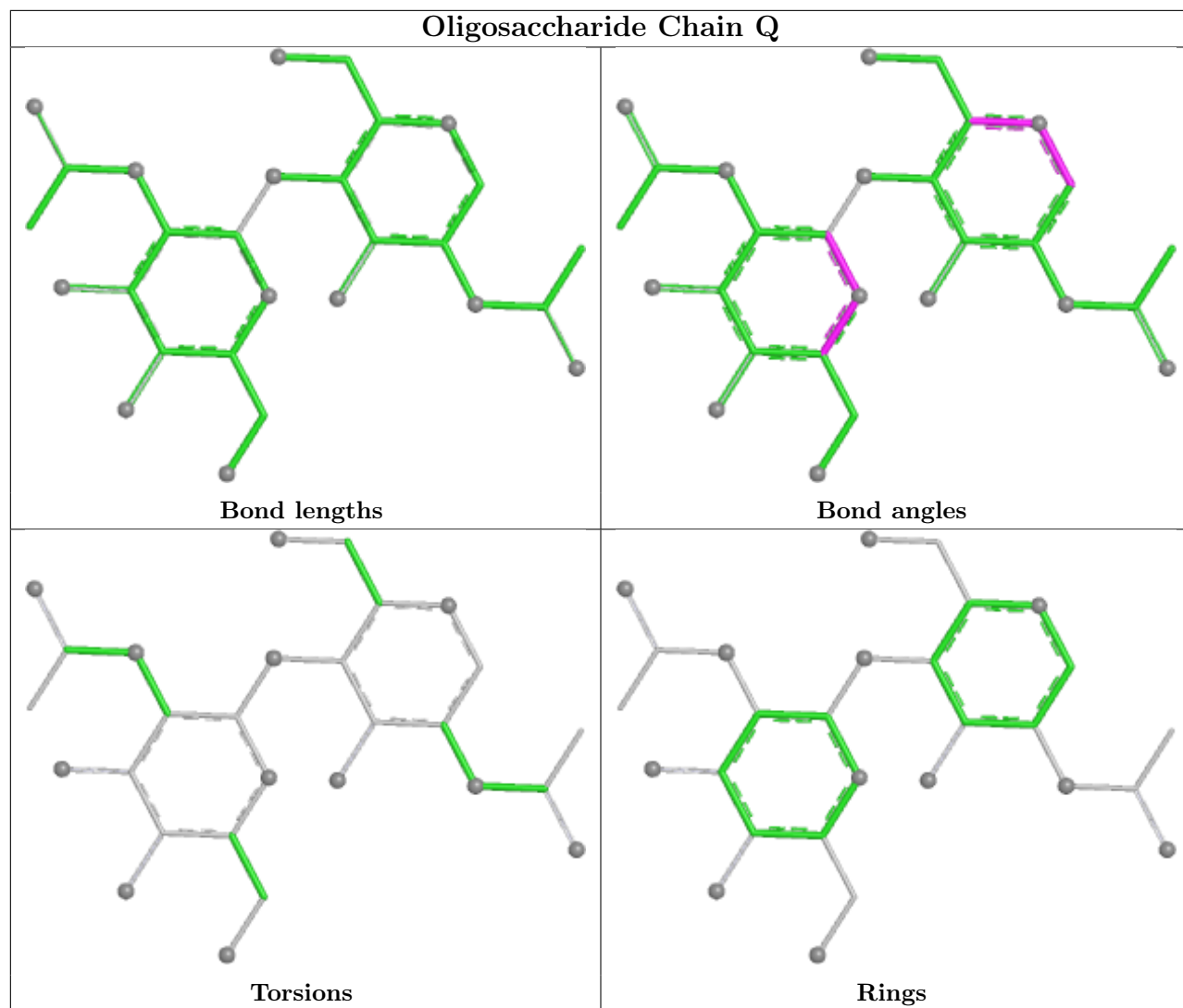




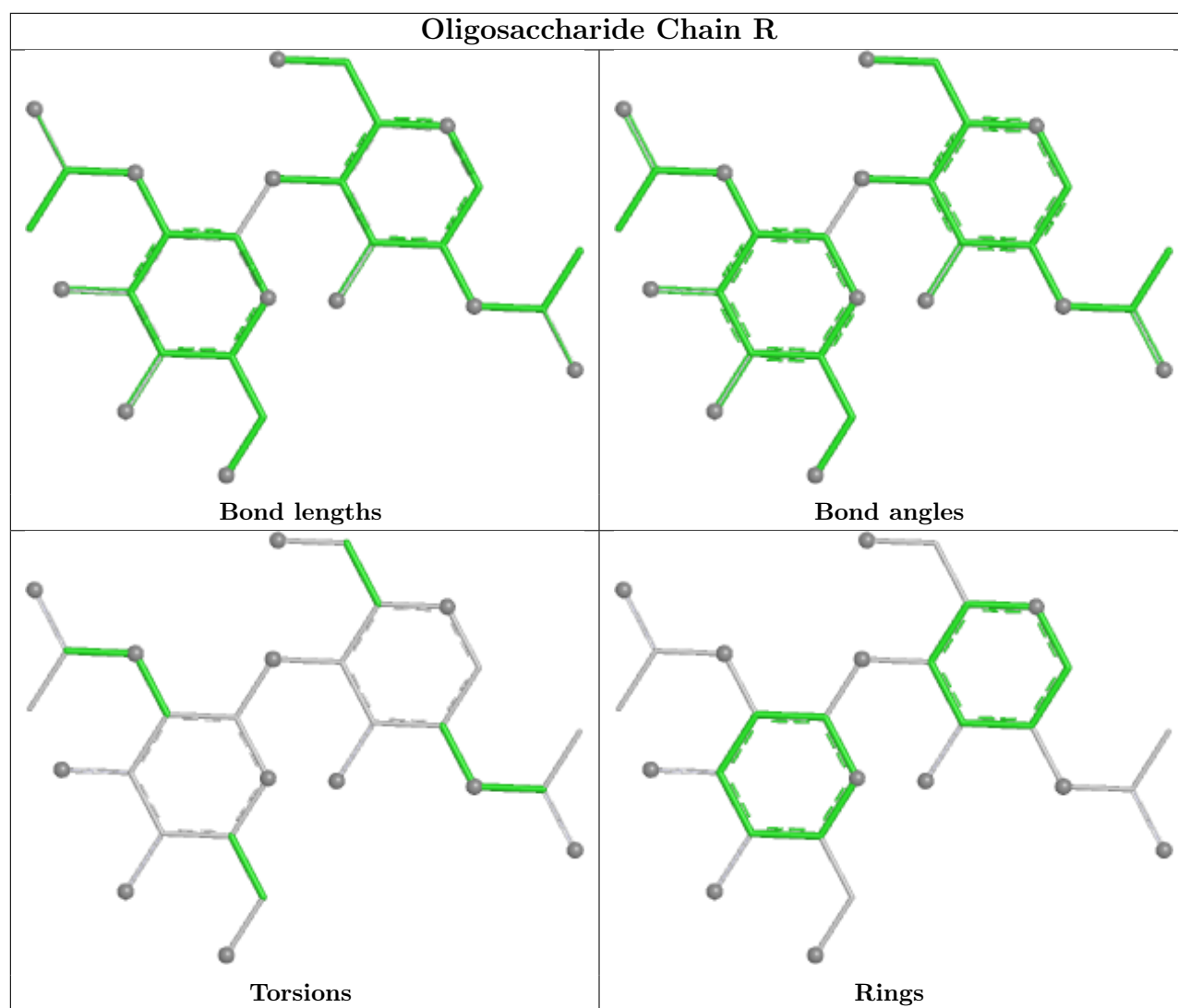




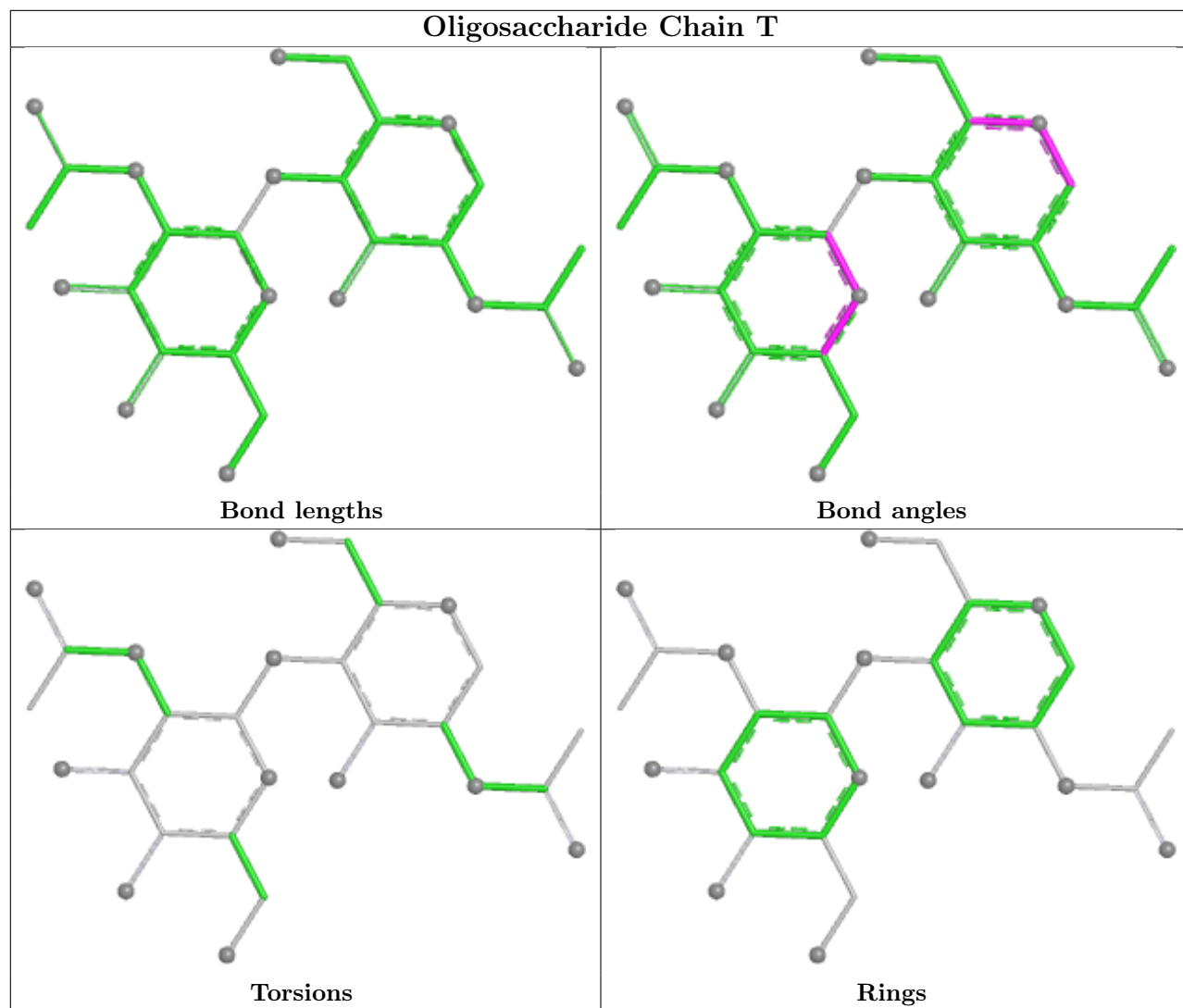




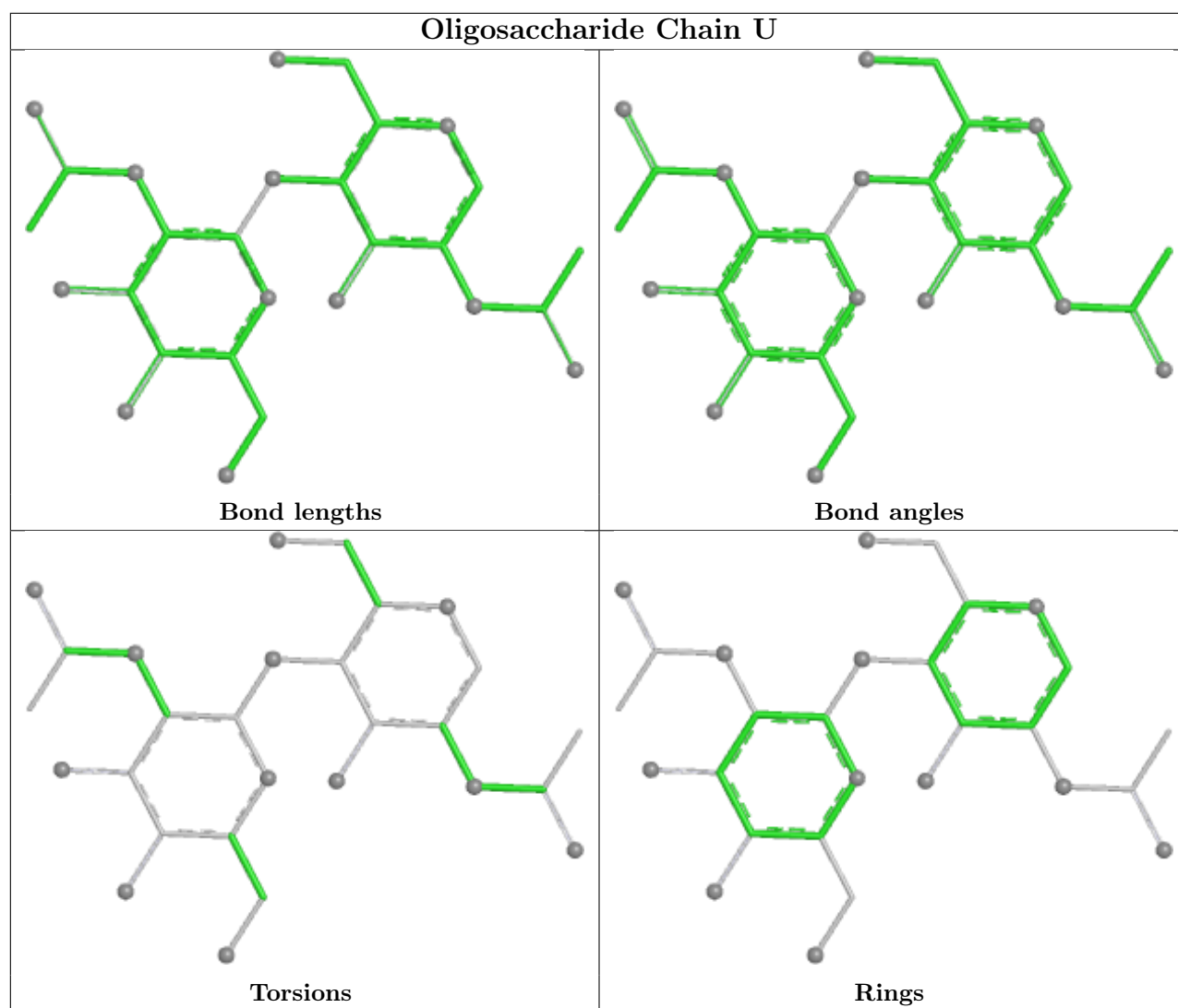




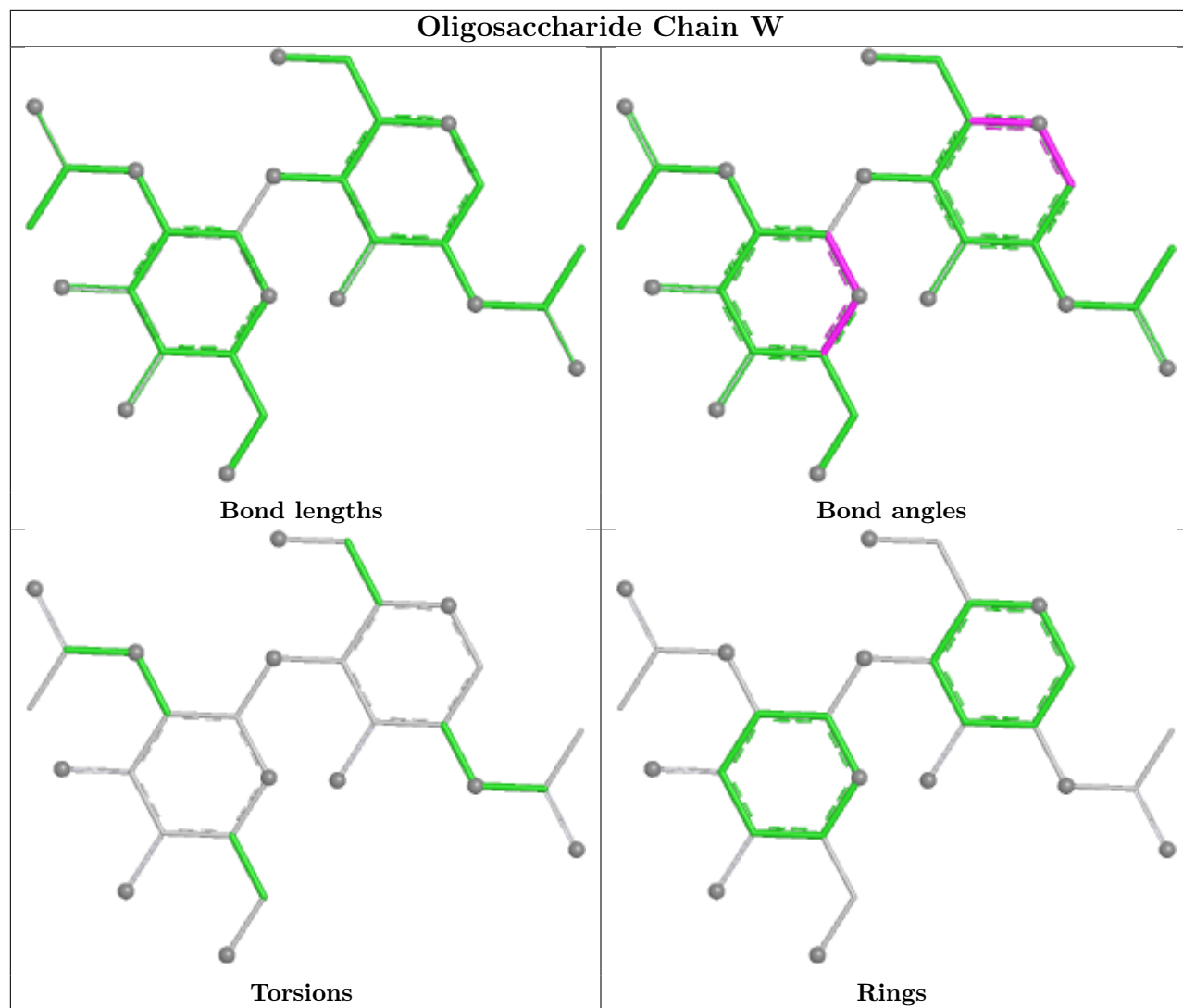




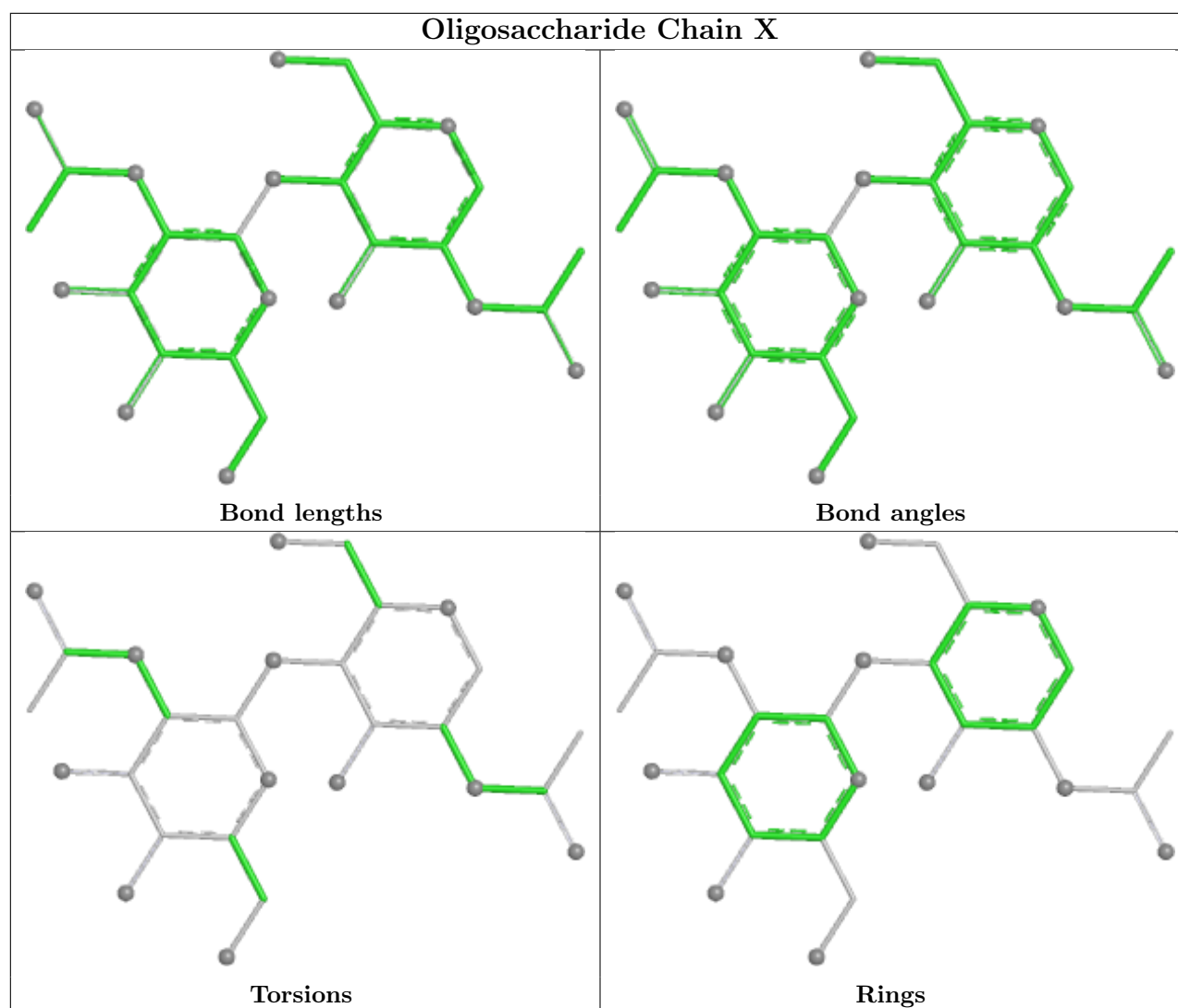












## 5.6 Ligand geometry [i](#)

12 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	0.67	0	17,19,21	0.98	1 (5%)
8	NAG	A	803	1	14,14,15	0.67	0	17,19,21	0.92	1 (5%)
8	NAG	A	804	1	14,14,15	0.72	0	17,19,21	0.81	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	0.69	0	17,19,21	0.94	1 (5%)
8	NAG	B	802	1	14,14,15	0.68	0	17,19,21	0.95	1 (5%)
8	NAG	C	801	1	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
8	NAG	C	802	1	14,14,15	0.68	0	17,19,21	0.94	1 (5%)
8	NAG	B	803	1	14,14,15	0.67	0	17,19,21	0.96	2 (11%)
8	NAG	C	804	1	14,14,15	0.71	0	17,19,21	0.81	0
8	NAG	C	803	1	14,14,15	0.67	0	17,19,21	0.93	1 (5%)
8	NAG	B	804	1	14,14,15	0.73	0	17,19,21	0.84	0
8	NAG	B	801	1	14,14,15	0.68	0	17,19,21	0.99	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	801	1	-	0/6/23/26	0/1/1/1
8	NAG	A	803	1	-	2/6/23/26	0/1/1/1
8	NAG	A	804	1	-	2/6/23/26	0/1/1/1
8	NAG	A	802	1	-	0/6/23/26	0/1/1/1
8	NAG	B	802	1	-	0/6/23/26	0/1/1/1
8	NAG	C	801	1	-	0/6/23/26	0/1/1/1
8	NAG	C	802	1	-	0/6/23/26	0/1/1/1
8	NAG	B	803	1	-	2/6/23/26	0/1/1/1
8	NAG	C	804	1	-	2/6/23/26	0/1/1/1
8	NAG	C	803	1	-	2/6/23/26	0/1/1/1
8	NAG	B	804	1	-	2/6/23/26	0/1/1/1
8	NAG	B	801	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	802	NAG	C1-O5-C5	2.80	115.94	112.19
8	C	802	NAG	C1-O5-C5	2.77	115.90	112.19
8	A	802	NAG	C1-O5-C5	2.75	115.88	112.19
8	C	801	NAG	C2-N2-C7	2.61	126.39	122.90
8	A	801	NAG	C2-N2-C7	2.60	126.38	122.90
8	B	801	NAG	C2-N2-C7	2.60	126.38	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	803	NAG	C1-O5-C5	2.12	115.03	112.19
8	B	803	NAG	C2-N2-C7	2.11	125.73	122.90
8	B	803	NAG	C1-O5-C5	2.10	115.01	112.19
8	A	803	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	803	NAG	C8-C7-N2-C2
8	A	803	NAG	O7-C7-N2-C2
8	A	804	NAG	C8-C7-N2-C2
8	A	804	NAG	O7-C7-N2-C2
8	B	803	NAG	C8-C7-N2-C2
8	B	803	NAG	O7-C7-N2-C2
8	B	804	NAG	C8-C7-N2-C2
8	B	804	NAG	O7-C7-N2-C2
8	C	803	NAG	C8-C7-N2-C2
8	C	803	NAG	O7-C7-N2-C2
8	C	804	NAG	C8-C7-N2-C2
8	C	804	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



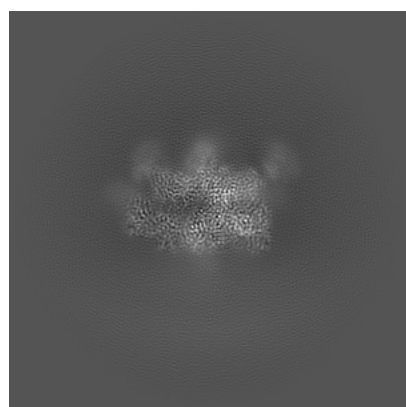
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43672. These allow visual inspection of the internal detail of the map and identification of artifacts.

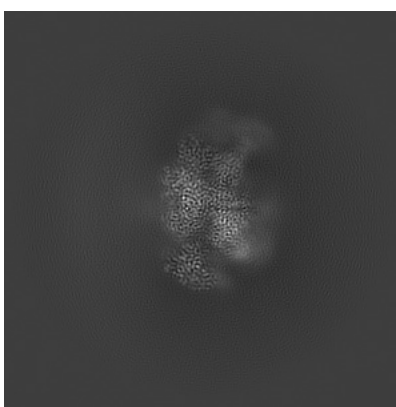
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

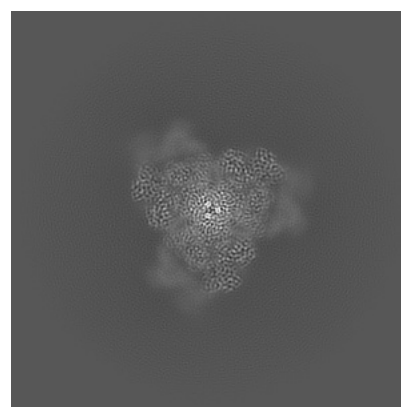
#### 6.1.1 Primary map



X



Y

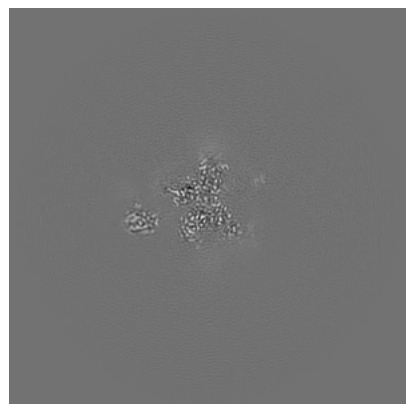


Z

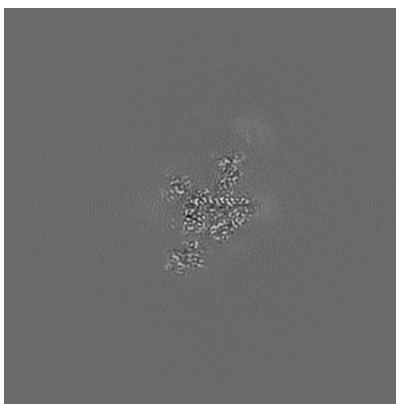
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

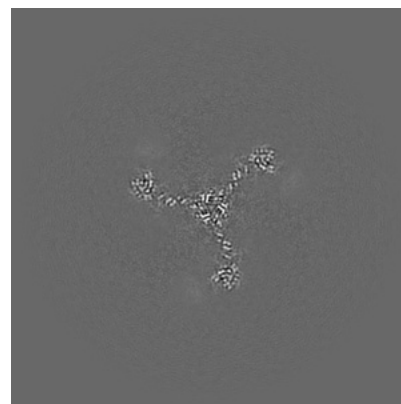
#### 6.2.1 Primary map



X Index: 240



Y Index: 240



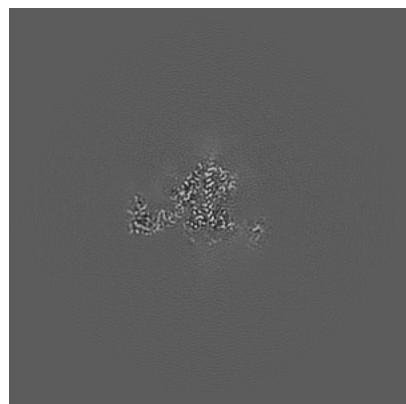
Z Index: 240



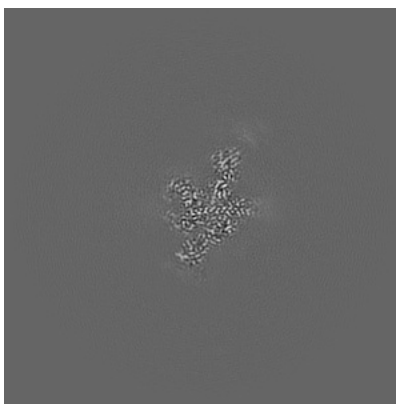
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

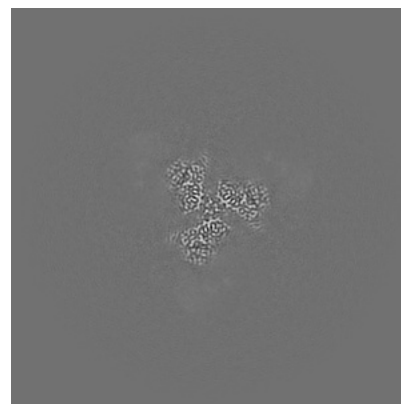
### 6.3.1 Primary map



X Index: 249



Y Index: 247

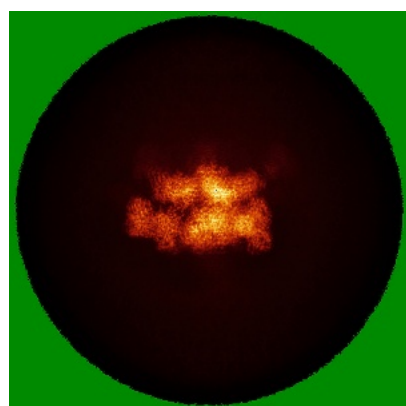


Z Index: 264

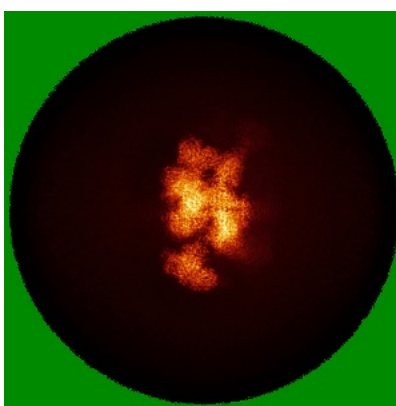
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

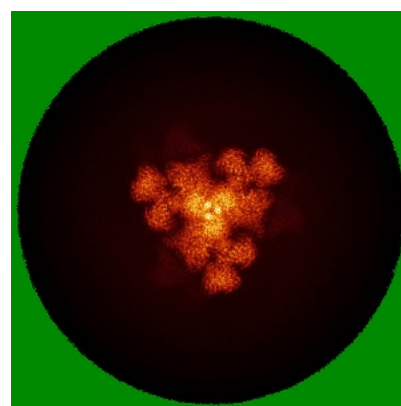
### 6.4.1 Primary map



X



Y



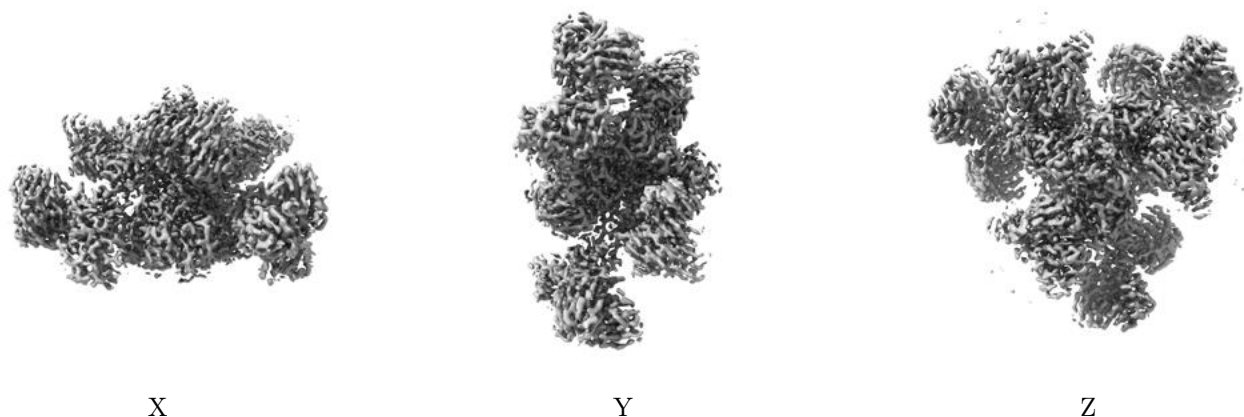
Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

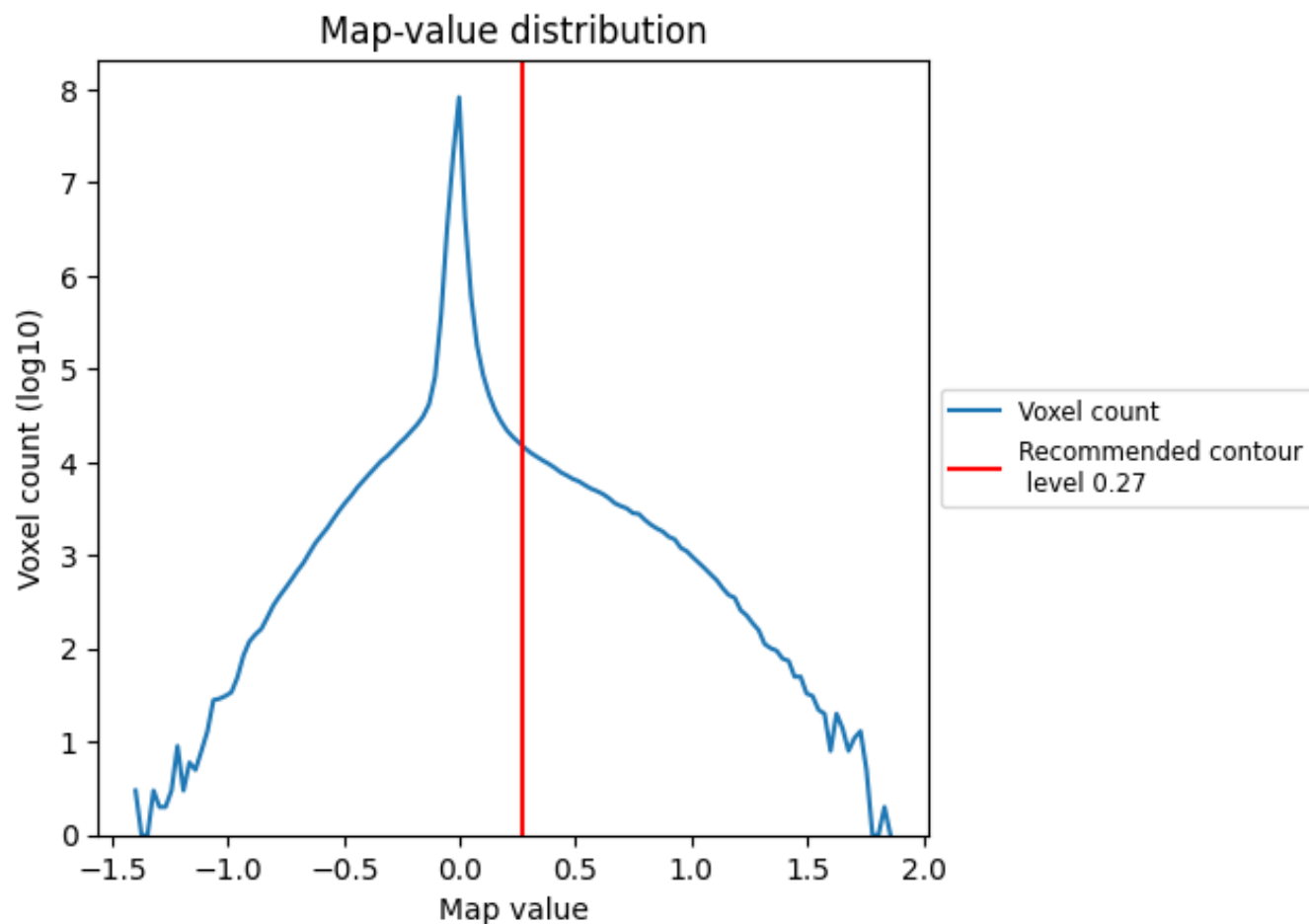
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

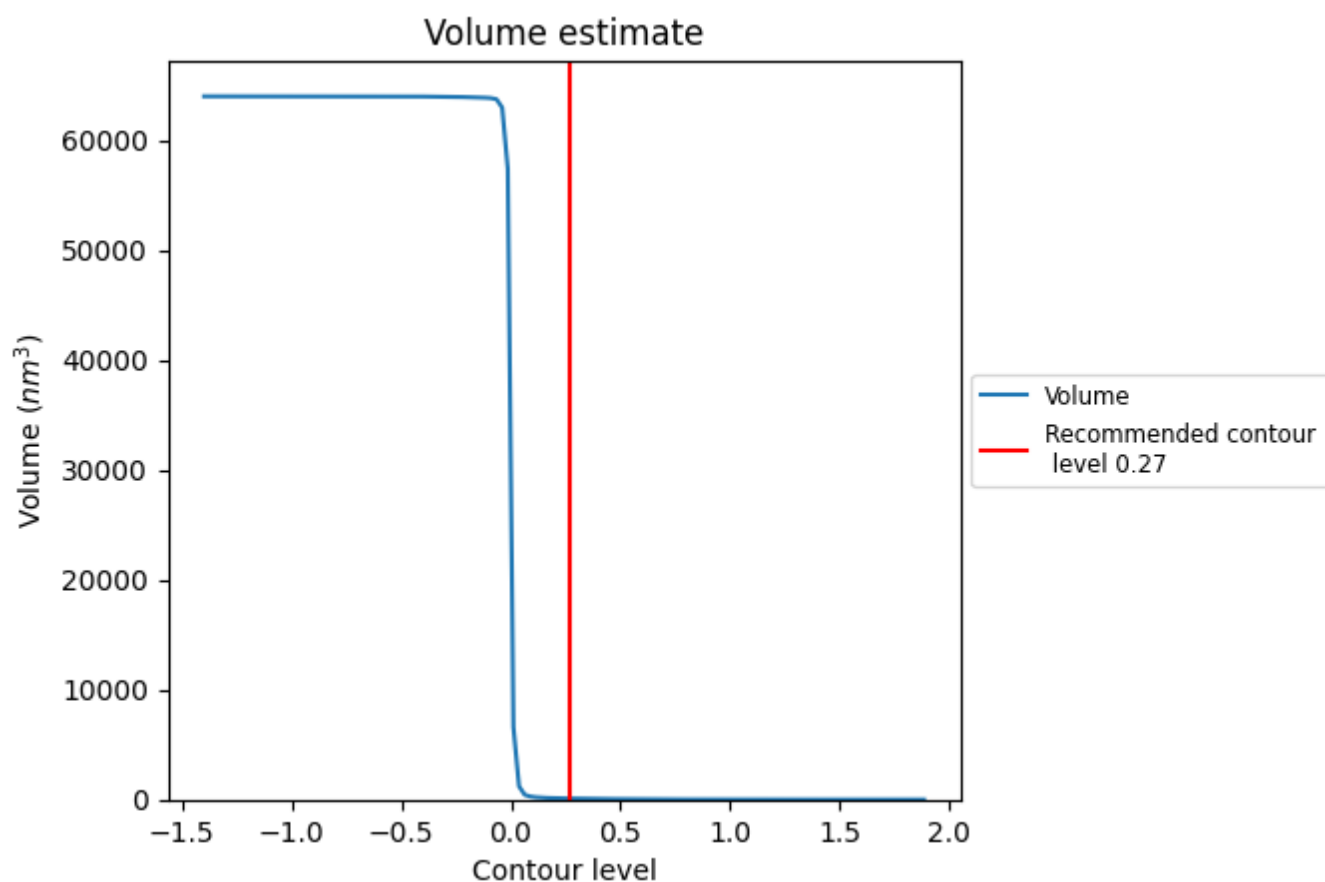
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

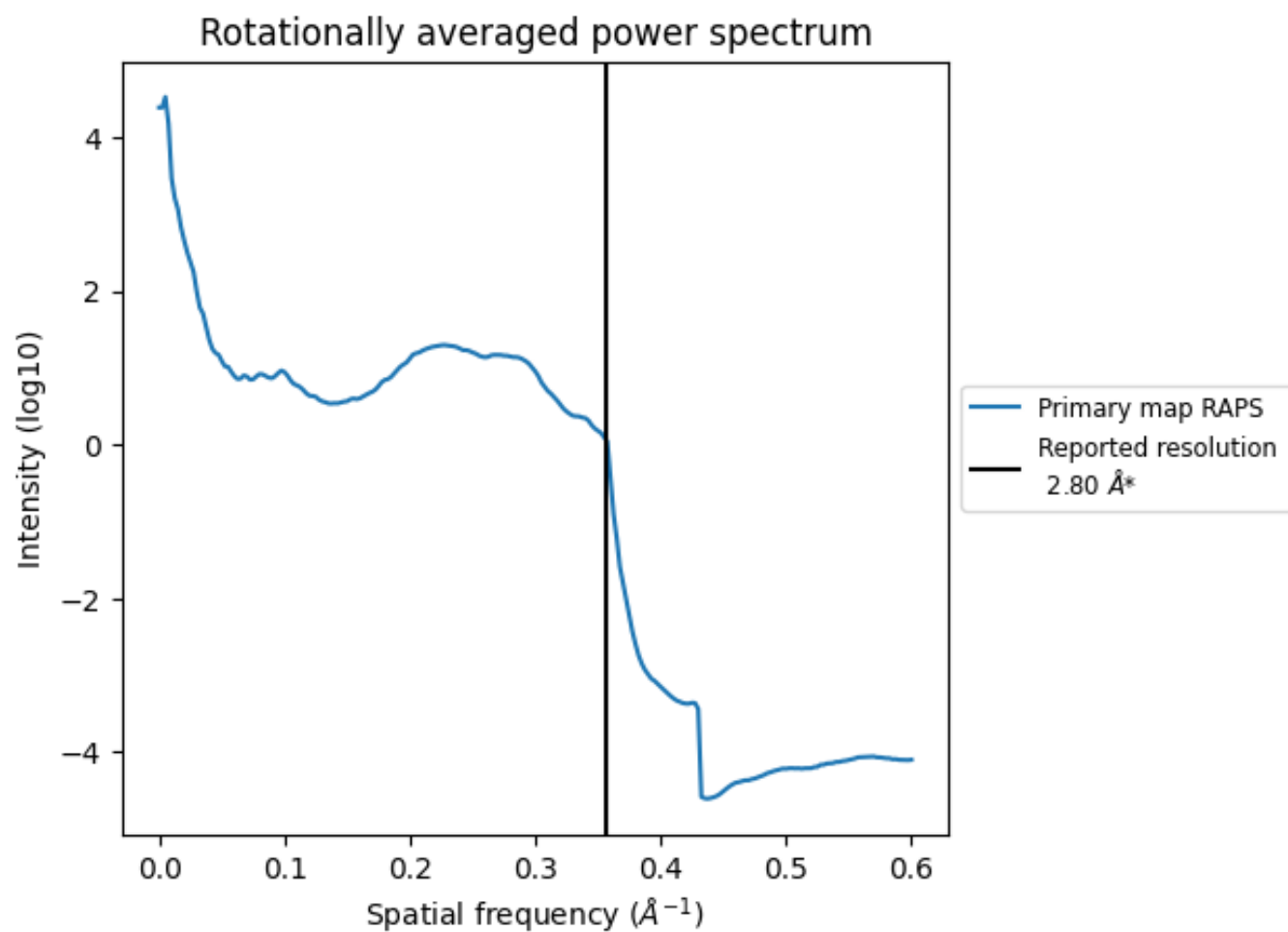


The volume at the recommended contour level is 94 nm<sup>3</sup>; this corresponds to an approximate mass of 84 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

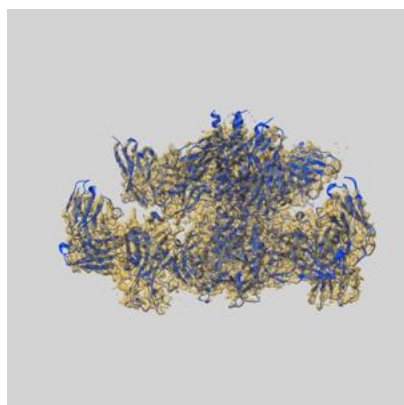
This section was not generated. No FSC curve or half-maps provided.



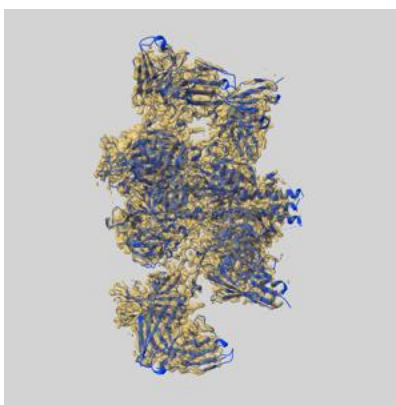
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43672 and PDB model 8VYN. Per-residue inclusion information can be found in section [3](#) on page [14](#).

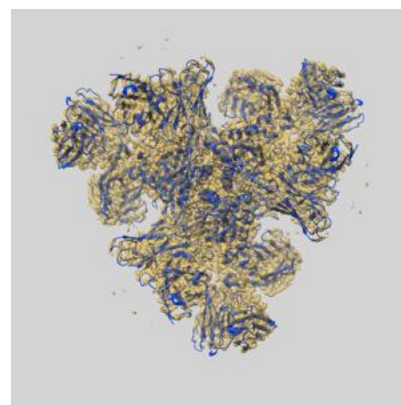
### 9.1 Map-model overlay [i](#)



X



Y

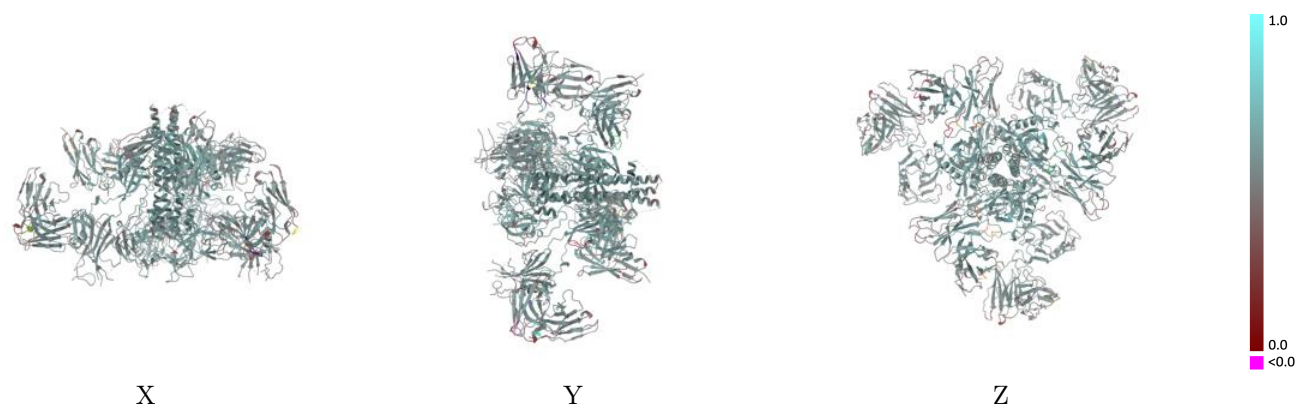


Z

The images above show the 3D surface view of the map at the recommended contour level 0.27 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](#)



The images above show the model with each residue coloured according to 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.

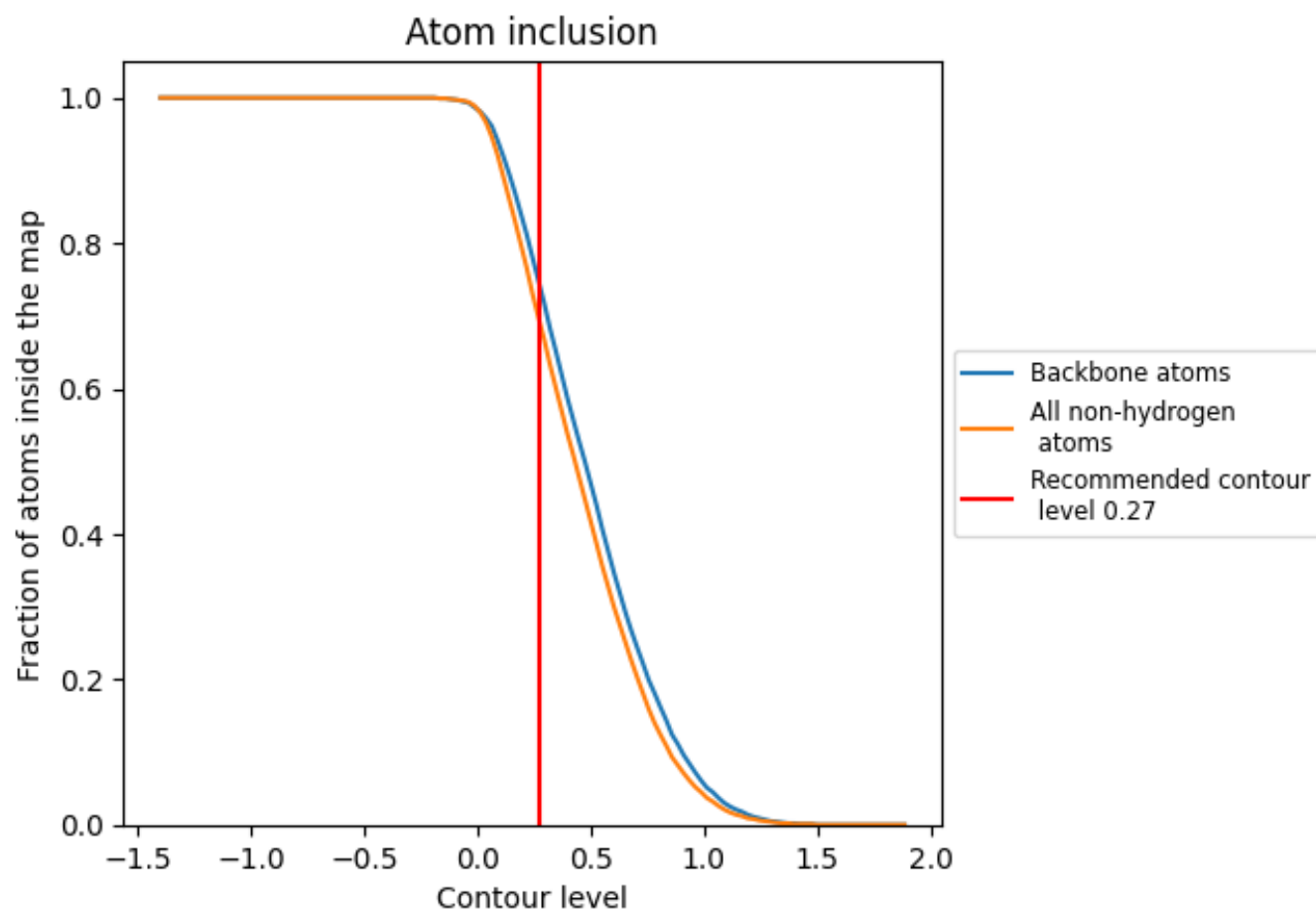
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.27).



## 9.4 Atom inclusion [i](#)





















































At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6960	 0.5510
A	 0.7420	 0.5690
B	 0.7400	 0.5700
C	 0.7400	 0.5700
D	 0.6870	 0.5610
E	 0.6680	 0.5380
F	 0.6290	 0.5140
G	 0.5940	 0.5030
H	 0.6870	 0.5610
I	 0.6690	 0.5430
J	 0.6290	 0.5140
K	 0.5900	 0.5000
L	 0.6890	 0.5610
M	 0.6650	 0.5410
N	 0.6310	 0.5160
O	 0.5910	 0.4990
P	 0.5900	 0.4700
Q	 0.5710	 0.4680
R	 0.4640	 0.5090
S	 0.5900	 0.4750
T	 0.5710	 0.4700
U	 0.4290	 0.5180
V	 0.5900	 0.4750
W	 0.5710	 0.4750
X	 0.3930	 0.5100

