Full wwPDB EM Validation Report ⓘ

Nov 21, 2024 – 12:13 PM EST

PDB ID	:	9BU6
EMDB ID	:	EMD-44901
Title	:	Vaccine elicited Fab C968.180 with influenza H10 JD13 HA trimer
Authors	:	Gorman, J.; Kwong, P.D.
Deposited on	:	2024-05-16
Resolution	:	3.65 Å(reported)
Based on initial model	:	.

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

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

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

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

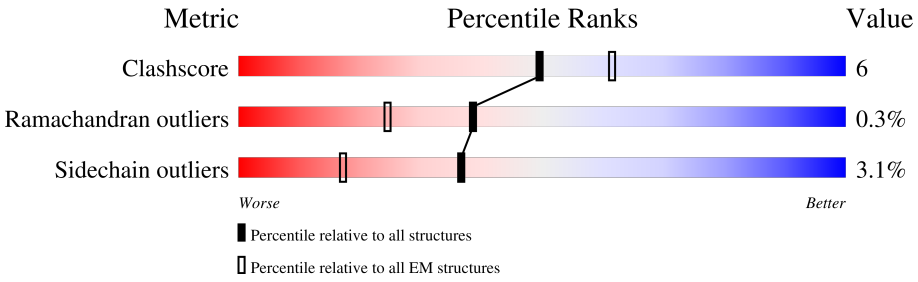
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.65 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	131	84% 15%
1	E	131	83% 15%
1	I	131	89% 8%
2	B	108	6% 87% 12%
2	F	108	6% 86% 13%
2	J	108	8% 91% 8%
3	C	325	85% 13%
3	G	325	82% 16%

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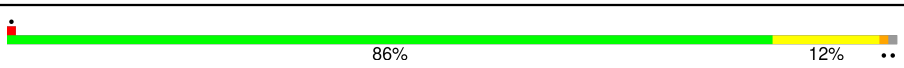
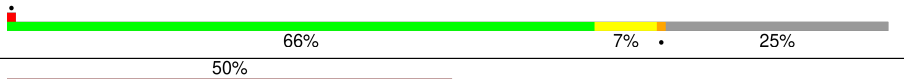
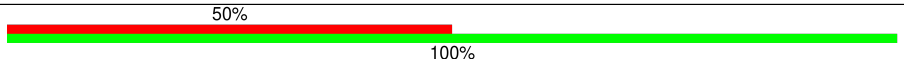
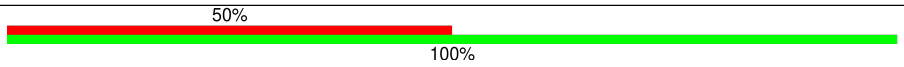
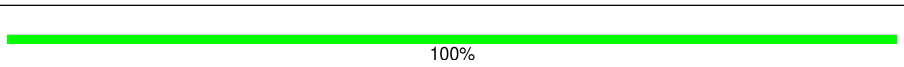
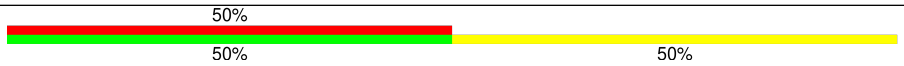
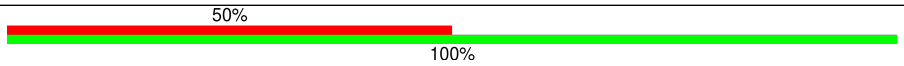
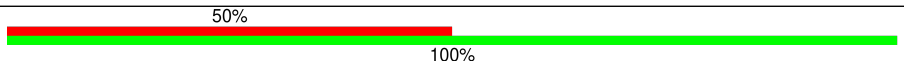
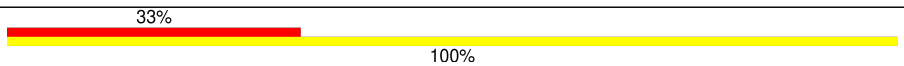
Mol	Chain	Length	Quality of chain
3	K	325	
4	D	230	
4	H	230	
4	L	230	
5	M	2	
5	N	2	
5	P	2	
5	Q	2	
5	S	2	
5	T	2	
6	O	3	
6	R	3	
6	U	3	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17439 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 Fab C968.180 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	129	Total	C	N	O	S	0	0
			1018	644	178	192	4		
1	E	129	Total	C	N	O	S	0	0
			1018	644	178	192	4		
1	I	129	Total	C	N	O	S	0	0
			1018	644	178	192	4		

- Molecule 2 is a protein called Fab C968.180 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	108	Total	C	N	O	S	0	0
			831	522	145	162	2		
2	F	108	Total	C	N	O	S	0	0
			831	522	145	162	2		
2	J	108	Total	C	N	O	S	0	0
			831	522	145	162	2		

- Molecule 3 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	322	Total	C	N	O	S	0	0
			2465	1526	453	469	17		
3	G	322	Total	C	N	O	S	0	0
			2465	1526	453	469	17		
3	K	322	Total	C	N	O	S	0	0
			2465	1526	453	469	17		

- Molecule 4 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	172	Total	C	N	O	S	0	0
			1390	860	240	282	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	172	Total	C	N	O	S	0	0
			1390	860	240	282	8		
4	L	172	Total	C	N	O	S	0	0
			1390	860	240	282	8		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	178	GLY	-	expression tag	UNP A0A0B4UV34
D	179	SER	-	expression tag	UNP A0A0B4UV34
D	180	GLY	-	expression tag	UNP A0A0B4UV34
D	181	TYR	-	expression tag	UNP A0A0B4UV34
D	182	ILE	-	expression tag	UNP A0A0B4UV34
D	183	PRO	-	expression tag	UNP A0A0B4UV34
D	184	GLU	-	expression tag	UNP A0A0B4UV34
D	185	ALA	-	expression tag	UNP A0A0B4UV34
D	186	PRO	-	expression tag	UNP A0A0B4UV34
D	187	ARG	-	expression tag	UNP A0A0B4UV34
D	188	ASP	-	expression tag	UNP A0A0B4UV34
D	189	GLY	-	expression tag	UNP A0A0B4UV34
D	190	GLN	-	expression tag	UNP A0A0B4UV34
D	191	ALA	-	expression tag	UNP A0A0B4UV34
D	192	TYR	-	expression tag	UNP A0A0B4UV34
D	193	VAL	-	expression tag	UNP A0A0B4UV34
D	194	ARG	-	expression tag	UNP A0A0B4UV34
D	195	LYS	-	expression tag	UNP A0A0B4UV34
D	196	ASP	-	expression tag	UNP A0A0B4UV34
D	197	GLY	-	expression tag	UNP A0A0B4UV34
D	198	GLU	-	expression tag	UNP A0A0B4UV34
D	199	TRP	-	expression tag	UNP A0A0B4UV34
D	200	VAL	-	expression tag	UNP A0A0B4UV34
D	201	LEU	-	expression tag	UNP A0A0B4UV34
D	202	LEU	-	expression tag	UNP A0A0B4UV34
D	203	SER	-	expression tag	UNP A0A0B4UV34
D	204	THR	-	expression tag	UNP A0A0B4UV34
D	205	PHE	-	expression tag	UNP A0A0B4UV34
D	206	LEU	-	expression tag	UNP A0A0B4UV34
D	207	GLY	-	expression tag	UNP A0A0B4UV34
D	208	SER	-	expression tag	UNP A0A0B4UV34
D	209	GLY	-	expression tag	UNP A0A0B4UV34
D	210	LEU	-	expression tag	UNP A0A0B4UV34
D	211	ASN	-	expression tag	UNP A0A0B4UV34

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Chain	Residue	Modelled	Actual	Comment	Reference
D	212	ASP	-	expression tag	UNP A0A0B4UV34
D	213	ILE	-	expression tag	UNP A0A0B4UV34
D	214	PHE	-	expression tag	UNP A0A0B4UV34
D	215	GLU	-	expression tag	UNP A0A0B4UV34
D	216	ALA	-	expression tag	UNP A0A0B4UV34
D	217	GLN	-	expression tag	UNP A0A0B4UV34
D	218	LYS	-	expression tag	UNP A0A0B4UV34
D	219	ILE	-	expression tag	UNP A0A0B4UV34
D	220	GLU	-	expression tag	UNP A0A0B4UV34
D	221	TRP	-	expression tag	UNP A0A0B4UV34
D	222	HIS	-	expression tag	UNP A0A0B4UV34
D	223	GLU	-	expression tag	UNP A0A0B4UV34
D	224	GLY	-	expression tag	UNP A0A0B4UV34
D	225	HIS	-	expression tag	UNP A0A0B4UV34
D	226	HIS	-	expression tag	UNP A0A0B4UV34
D	227	HIS	-	expression tag	UNP A0A0B4UV34
D	228	HIS	-	expression tag	UNP A0A0B4UV34
D	229	HIS	-	expression tag	UNP A0A0B4UV34
D	230	HIS	-	expression tag	UNP A0A0B4UV34
H	178	GLY	-	expression tag	UNP A0A0B4UV34
H	179	SER	-	expression tag	UNP A0A0B4UV34
H	180	GLY	-	expression tag	UNP A0A0B4UV34
H	181	TYR	-	expression tag	UNP A0A0B4UV34
H	182	ILE	-	expression tag	UNP A0A0B4UV34
H	183	PRO	-	expression tag	UNP A0A0B4UV34
H	184	GLU	-	expression tag	UNP A0A0B4UV34
H	185	ALA	-	expression tag	UNP A0A0B4UV34
H	186	PRO	-	expression tag	UNP A0A0B4UV34
H	187	ARG	-	expression tag	UNP A0A0B4UV34
H	188	ASP	-	expression tag	UNP A0A0B4UV34
H	189	GLY	-	expression tag	UNP A0A0B4UV34
H	190	GLN	-	expression tag	UNP A0A0B4UV34
H	191	ALA	-	expression tag	UNP A0A0B4UV34
H	192	TYR	-	expression tag	UNP A0A0B4UV34
H	193	VAL	-	expression tag	UNP A0A0B4UV34
H	194	ARG	-	expression tag	UNP A0A0B4UV34
H	195	LYS	-	expression tag	UNP A0A0B4UV34
H	196	ASP	-	expression tag	UNP A0A0B4UV34
H	197	GLY	-	expression tag	UNP A0A0B4UV34
H	198	GLU	-	expression tag	UNP A0A0B4UV34
H	199	TRP	-	expression tag	UNP A0A0B4UV34
H	200	VAL	-	expression tag	UNP A0A0B4UV34

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Chain	Residue	Modelled	Actual	Comment	Reference
H	201	LEU	-	expression tag	UNP A0A0B4UV34
H	202	LEU	-	expression tag	UNP A0A0B4UV34
H	203	SER	-	expression tag	UNP A0A0B4UV34
H	204	THR	-	expression tag	UNP A0A0B4UV34
H	205	PHE	-	expression tag	UNP A0A0B4UV34
H	206	LEU	-	expression tag	UNP A0A0B4UV34
H	207	GLY	-	expression tag	UNP A0A0B4UV34
H	208	SER	-	expression tag	UNP A0A0B4UV34
H	209	GLY	-	expression tag	UNP A0A0B4UV34
H	210	LEU	-	expression tag	UNP A0A0B4UV34
H	211	ASN	-	expression tag	UNP A0A0B4UV34
H	212	ASP	-	expression tag	UNP A0A0B4UV34
H	213	ILE	-	expression tag	UNP A0A0B4UV34
H	214	PHE	-	expression tag	UNP A0A0B4UV34
H	215	GLU	-	expression tag	UNP A0A0B4UV34
H	216	ALA	-	expression tag	UNP A0A0B4UV34
H	217	GLN	-	expression tag	UNP A0A0B4UV34
H	218	LYS	-	expression tag	UNP A0A0B4UV34
H	219	ILE	-	expression tag	UNP A0A0B4UV34
H	220	GLU	-	expression tag	UNP A0A0B4UV34
H	221	TRP	-	expression tag	UNP A0A0B4UV34
H	222	HIS	-	expression tag	UNP A0A0B4UV34
H	223	GLU	-	expression tag	UNP A0A0B4UV34
H	224	GLY	-	expression tag	UNP A0A0B4UV34
H	225	HIS	-	expression tag	UNP A0A0B4UV34
H	226	HIS	-	expression tag	UNP A0A0B4UV34
H	227	HIS	-	expression tag	UNP A0A0B4UV34
H	228	HIS	-	expression tag	UNP A0A0B4UV34
H	229	HIS	-	expression tag	UNP A0A0B4UV34
H	230	HIS	-	expression tag	UNP A0A0B4UV34
L	178	GLY	-	expression tag	UNP A0A0B4UV34
L	179	SER	-	expression tag	UNP A0A0B4UV34
L	180	GLY	-	expression tag	UNP A0A0B4UV34
L	181	TYR	-	expression tag	UNP A0A0B4UV34
L	182	ILE	-	expression tag	UNP A0A0B4UV34
L	183	PRO	-	expression tag	UNP A0A0B4UV34
L	184	GLU	-	expression tag	UNP A0A0B4UV34
L	185	ALA	-	expression tag	UNP A0A0B4UV34
L	186	PRO	-	expression tag	UNP A0A0B4UV34
L	187	ARG	-	expression tag	UNP A0A0B4UV34
L	188	ASP	-	expression tag	UNP A0A0B4UV34
L	189	GLY	-	expression tag	UNP A0A0B4UV34

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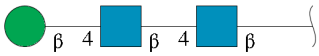
Chain	Residue	Modelled	Actual	Comment	Reference
L	190	GLN	-	expression tag	UNP A0A0B4UV34
L	191	ALA	-	expression tag	UNP A0A0B4UV34
L	192	TYR	-	expression tag	UNP A0A0B4UV34
L	193	VAL	-	expression tag	UNP A0A0B4UV34
L	194	ARG	-	expression tag	UNP A0A0B4UV34
L	195	LYS	-	expression tag	UNP A0A0B4UV34
L	196	ASP	-	expression tag	UNP A0A0B4UV34
L	197	GLY	-	expression tag	UNP A0A0B4UV34
L	198	GLU	-	expression tag	UNP A0A0B4UV34
L	199	TRP	-	expression tag	UNP A0A0B4UV34
L	200	VAL	-	expression tag	UNP A0A0B4UV34
L	201	LEU	-	expression tag	UNP A0A0B4UV34
L	202	LEU	-	expression tag	UNP A0A0B4UV34
L	203	SER	-	expression tag	UNP A0A0B4UV34
L	204	THR	-	expression tag	UNP A0A0B4UV34
L	205	PHE	-	expression tag	UNP A0A0B4UV34
L	206	LEU	-	expression tag	UNP A0A0B4UV34
L	207	GLY	-	expression tag	UNP A0A0B4UV34
L	208	SER	-	expression tag	UNP A0A0B4UV34
L	209	GLY	-	expression tag	UNP A0A0B4UV34
L	210	LEU	-	expression tag	UNP A0A0B4UV34
L	211	ASN	-	expression tag	UNP A0A0B4UV34
L	212	ASP	-	expression tag	UNP A0A0B4UV34
L	213	ILE	-	expression tag	UNP A0A0B4UV34
L	214	PHE	-	expression tag	UNP A0A0B4UV34
L	215	GLU	-	expression tag	UNP A0A0B4UV34
L	216	ALA	-	expression tag	UNP A0A0B4UV34
L	217	GLN	-	expression tag	UNP A0A0B4UV34
L	218	LYS	-	expression tag	UNP A0A0B4UV34
L	219	ILE	-	expression tag	UNP A0A0B4UV34
L	220	GLU	-	expression tag	UNP A0A0B4UV34
L	221	TRP	-	expression tag	UNP A0A0B4UV34
L	222	HIS	-	expression tag	UNP A0A0B4UV34
L	223	GLU	-	expression tag	UNP A0A0B4UV34
L	224	GLY	-	expression tag	UNP A0A0B4UV34
L	225	HIS	-	expression tag	UNP A0A0B4UV34
L	226	HIS	-	expression tag	UNP A0A0B4UV34
L	227	HIS	-	expression tag	UNP A0A0B4UV34
L	228	HIS	-	expression tag	UNP A0A0B4UV34
L	229	HIS	-	expression tag	UNP A0A0B4UV34
L	230	HIS	-	expression tag	UNP A0A0B4UV34

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

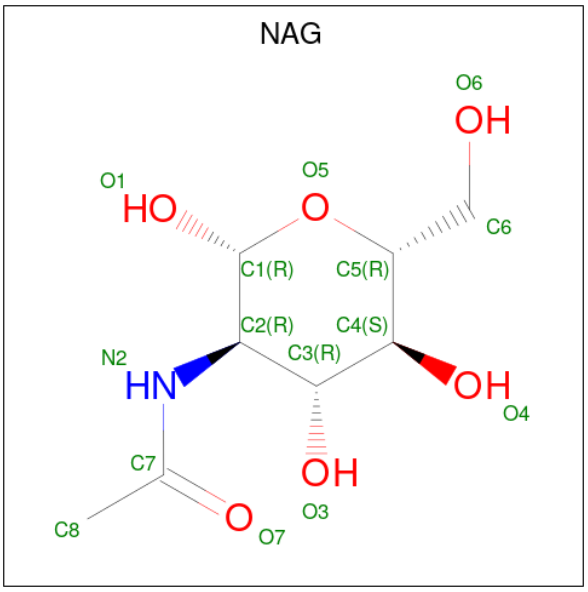
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	O	3	Total	C	N	O	0	0
			39	22	2	15		
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	U	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



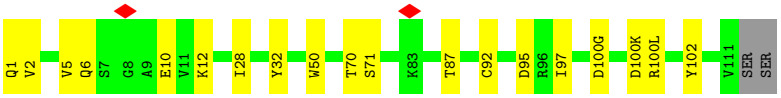
Mol	Chain	Residues	Atoms	AltConf
7	D	1	Total C N O 14 8 1 5	0
7	H	1	Total C N O 14 8 1 5	0
7	L	1	Total C N O 14 8 1 5	0

3 Residue-property plots (i)

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

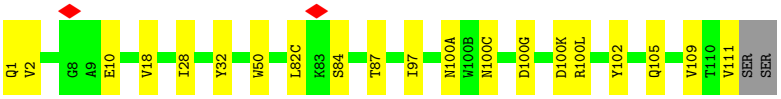
• Molecule 1: Fab C968.180 heavy chain

Chain A:



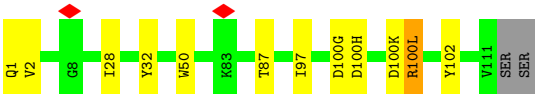
• Molecule 1: Fab C968.180 heavy chain

Chain E:



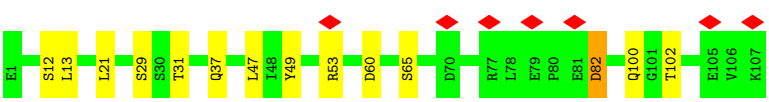
• Molecule 1: Fab C968.180 heavy chain

Chain I:



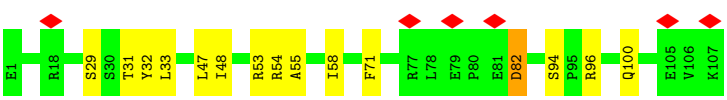
• Molecule 2: Fab C968.180 light chain

Chain B:



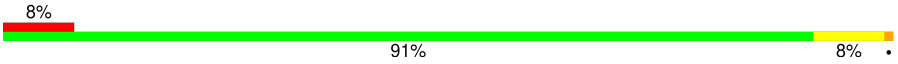
• Molecule 2: Fab C968.180 light chain

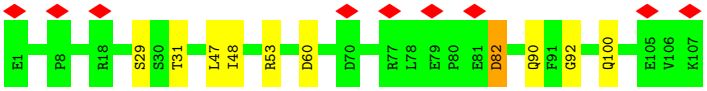
Chain F:



• Molecule 2: Fab C968.180 light chain

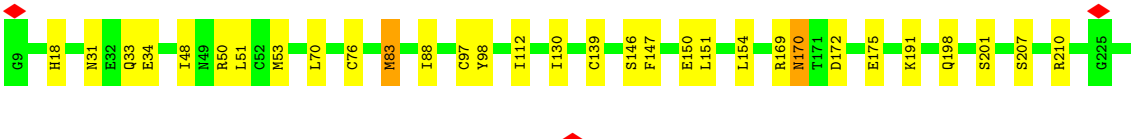
Chain J:





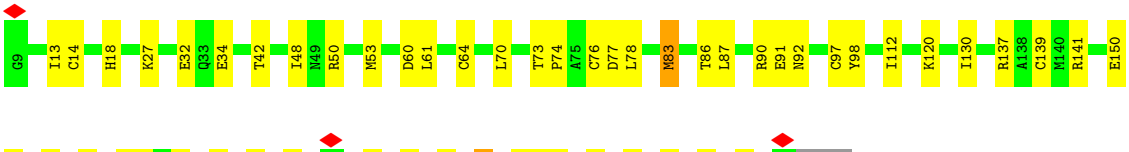
• Molecule 3: Hemagglutinin HA1

Chain C:



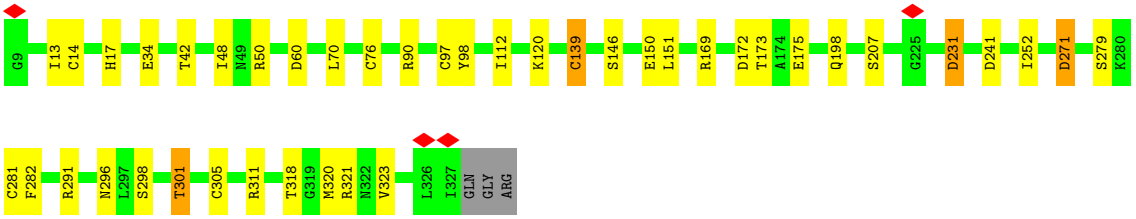
• Molecule 3: Hemagglutinin HA1

Chain G:



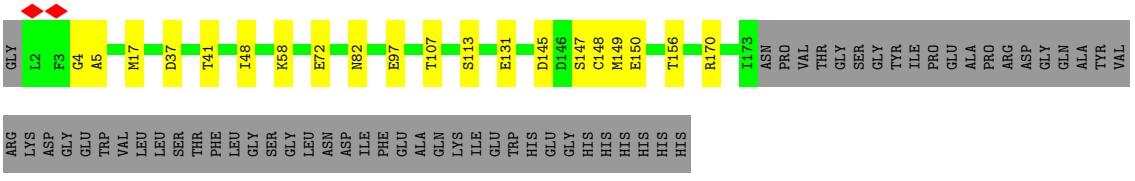
• Molecule 3: Hemagglutinin HA1

Chain K:



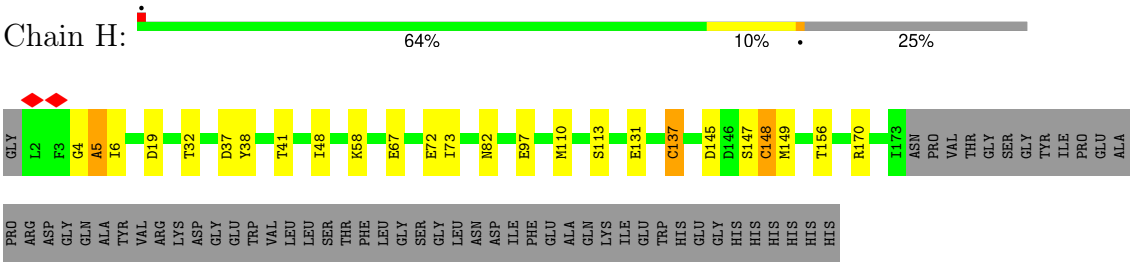
• Molecule 4: Hemagglutinin HA2

Chain D:



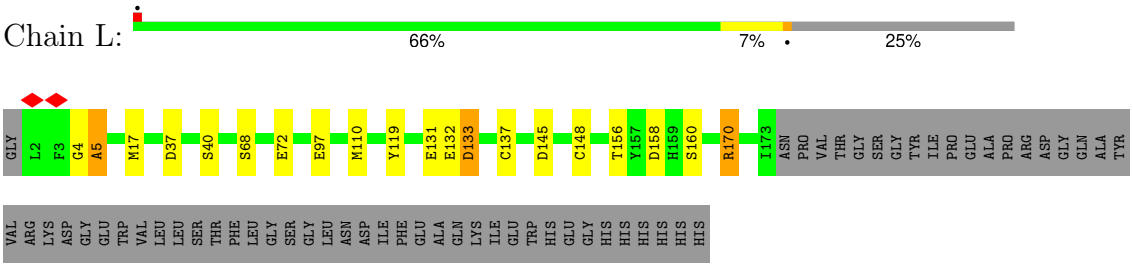
• Molecule 4: Hemagglutinin HA2

Chain H:



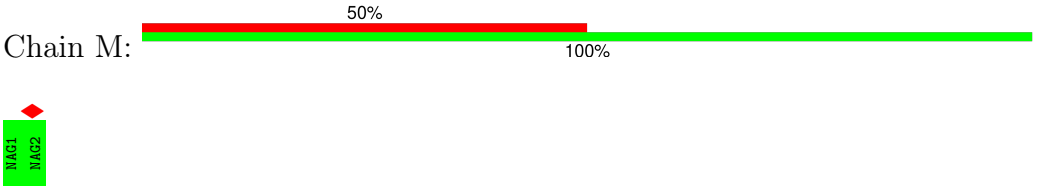
• Molecule 4: Hemagglutinin HA2

Chain L:



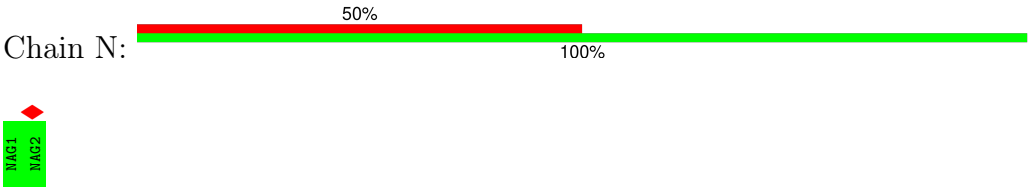
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



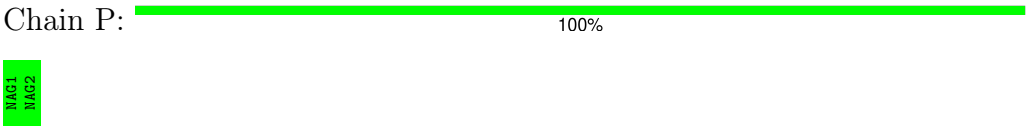
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain P:



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

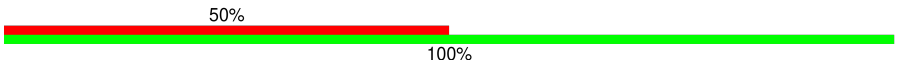
Chain Q:

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

Chain S:

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

Chain T:



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

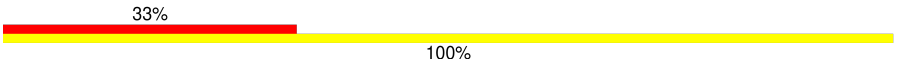
Chain O:

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

Chain R:

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

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.153	Depositor
Minimum map value	-1.594	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	346.56, 346.56, 346.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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	0.28	0/1045	0.52	0/1418
1	E	0.30	0/1045	0.57	0/1418
1	I	0.30	0/1045	0.58	0/1418
2	B	0.27	0/851	0.56	0/1152
2	F	0.30	0/851	0.55	0/1152
2	J	0.27	0/851	0.56	0/1152
3	C	0.26	0/2514	0.53	0/3406
3	G	0.27	0/2514	0.53	0/3406
3	K	0.26	0/2514	0.53	0/3406
4	D	0.27	0/1415	0.49	0/1910
4	H	0.28	0/1415	0.57	3/1910 (0.2%)
4	L	0.28	0/1415	0.51	0/1910
All	All	0.28	0/17475	0.54	3/23658 (0.0%)

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
2	F	0	2
4	D	0	1
4	H	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	32	THR	N-CA-CB	8.59	126.61	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	137	CYS	CA-CB-SG	6.54	125.78	114.00
4	H	32	THR	N-CA-C	-5.97	94.88	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	82	ASN	Peptide
2	F	53	ARG	Sidechain
2	F	54	ARG	Sidechain
4	H	82	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1018	0	969	14	0
1	E	1018	0	969	10	0
1	I	1018	0	969	10	0
2	B	831	0	810	12	0
2	F	831	0	810	9	0
2	J	831	0	810	7	0
3	C	2465	0	2421	26	0
3	G	2465	0	2421	36	0
3	K	2465	0	2421	30	0
4	D	1390	0	1288	11	0
4	H	1390	0	1288	15	0
4	L	1390	0	1288	12	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	1	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
6	O	39	0	34	1	0
6	R	39	0	34	3	0
6	U	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	14	0	13	1	0
7	H	14	0	13	0	0
7	L	14	0	13	0	0
All	All	17439	0	16755	189	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.

All (189) 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)
2:B:49:TYR:OH	2:B:53:ARG:HD3	1.66	0.94
4:L:119:TYR:OH	4:L:132:GLU:OE1	1.90	0.90
1:A:1:GLN:N	1:A:1:GLN:OE1	2.07	0.88
2:F:94:SER:OG	2:F:96:ARG:NH1	2.10	0.84
2:B:49:TYR:CZ	2:B:53:ARG:HD3	2.14	0.82
6:O:1:NAG:O7	6:O:1:NAG:O3	1.99	0.79
1:E:100(G):ASP:OD2	1:E:100(L):ARG:NH1	2.17	0.77
3:G:311:ARG:NH1	4:H:97:GLU:OE2	2.17	0.77
1:A:97:ILE:HD11	1:A:100(L):ARG:NH2	2.01	0.76
2:B:49:TYR:OH	2:B:53:ARG:CD	2.34	0.76
3:G:14:CYS:HA	4:H:137:CYS:HB3	1.69	0.74
6:R:1:NAG:O7	6:R:1:NAG:O3	2.02	0.73
1:I:1:GLN:N	1:I:1:GLN:OE1	2.20	0.72
3:G:175:GLU:N	3:G:175:GLU:OE1	2.22	0.72
3:G:60:ASP:OD1	3:G:90:ARG:NH1	2.23	0.72
3:K:175:GLU:N	3:K:175:GLU:OE1	2.23	0.72
3:C:175:GLU:N	3:C:175:GLU:OE1	2.23	0.71
4:L:37:ASP:OD2	4:L:40:SER:OG	2.09	0.71
1:E:1:GLN:OE1	1:E:1:GLN:N	2.20	0.71
3:K:296:ASN:ND2	3:K:311:ARG:O	2.25	0.70
3:K:14:CYS:HA	4:L:137:CYS:HB3	1.77	0.67
1:I:100(G):ASP:OD2	1:I:100(L):ARG:NH2	2.28	0.66
3:C:198:GLN:N	3:C:198:GLN:OE1	2.30	0.65
4:D:37:ASP:O	4:D:41:THR:HG22	1.96	0.65
3:G:172:ASP:OD1	3:G:173:THR:N	2.29	0.65
3:K:139:CYS:O	3:K:146:SER:OG	2.10	0.63
3:K:271:ASP:N	3:K:271:ASP:OD1	2.30	0.63
4:H:37:ASP:O	4:H:41:THR:HG22	1.99	0.63
3:G:130:ILE:HG21	3:G:154:LEU:HD23	1.80	0.63
3:G:271:ASP:N	3:G:271:ASP:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:48:ILE:HD11	4:H:110:MET:CE	2.30	0.62
3:C:51:LEU:HD21	3:C:268:ILE:HD11	1.82	0.61
3:C:172:ASP:OD2	3:C:259:LYS:NZ	2.33	0.61
4:H:156:THR:HG22	4:H:156:THR:O	2.00	0.60
3:C:271:ASP:N	3:C:271:ASP:OD1	2.36	0.59
4:L:156:THR:HG22	4:L:156:THR:O	2.01	0.59
3:G:77:ASP:OD2	3:G:141:ARG:NH1	2.34	0.58
1:E:2:VAL:HG11	1:E:102:TYR:CD1	2.39	0.58
4:H:148:CYS:SG	4:H:149:MET:N	2.76	0.58
3:C:301:THR:OG1	3:C:305:CYS:SG	2.55	0.58
1:A:28:ILE:N	1:A:28:ILE:HD12	2.19	0.58
4:D:156:THR:HG22	4:D:156:THR:O	2.04	0.58
1:E:10:GLU:HB3	1:E:109:VAL:HG22	1.85	0.57
1:E:28:ILE:H	1:E:28:ILE:HD12	1.69	0.57
3:K:172:ASP:OD1	3:K:173:THR:N	2.35	0.57
2:B:49:TYR:CE1	2:B:53:ARG:HD3	2.39	0.57
3:K:60:ASP:OD1	3:K:90:ARG:NH1	2.38	0.57
3:C:170:ASN:OD1	3:C:240:GLY:N	2.35	0.57
3:G:207:SER:OG	3:G:241:ASP:OD2	2.22	0.57
3:G:14:CYS:HA	4:H:137:CYS:CB	2.35	0.57
2:B:49:TYR:OH	2:B:53:ARG:NE	2.39	0.56
1:I:97:ILE:HD11	1:I:100(L):ARG:NH2	2.20	0.56
4:H:19:ASP:OD1	4:H:38:TYR:OH	2.20	0.56
3:G:231:ASP:OD1	3:G:231:ASP:N	2.36	0.55
4:H:48:ILE:HD11	4:H:110:MET:HE2	1.87	0.55
1:A:97:ILE:HD11	1:A:100(L):ARG:CZ	2.36	0.55
3:K:318:THR:HG22	3:K:318:THR:O	2.06	0.55
2:J:90:GLN:OE1	2:J:92:GLY:N	2.34	0.54
1:A:28:ILE:HD12	1:A:28:ILE:H	1.73	0.54
4:L:131:GLU:OE2	4:L:170:ARG:NH1	2.41	0.54
3:G:277:CYS:SG	3:G:278:GLU:N	2.81	0.54
3:C:207:SER:OG	3:C:241:ASP:OD2	2.27	0.53
1:A:2:VAL:HG11	1:A:102:TYR:HD2	1.73	0.53
3:K:207:SER:OG	3:K:241:ASP:OD2	2.27	0.53
3:C:252:ILE:HG22	3:C:252:ILE:O	2.09	0.52
4:D:58:LYS:NZ	4:L:97:GLU:OE2	2.42	0.52
3:G:323:VAL:O	3:G:323:VAL:HG13	2.09	0.52
3:K:14:CYS:HA	4:L:137:CYS:CB	2.38	0.52
4:D:97:GLU:OE2	4:H:58:LYS:NZ	2.43	0.52
4:D:148:CYS:SG	4:D:149:MET:N	2.82	0.52
1:A:10:GLU:OE2	1:A:12:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:VAL:HG11	1:I:102:TYR:CD2	2.45	0.52
3:G:120:LYS:NZ	3:G:150:GLU:OE1	2.41	0.51
1:A:2:VAL:HG11	1:A:102:TYR:CD2	2.46	0.51
3:G:169:ARG:NH1	5:Q:1:NAG:O5	2.44	0.50
3:C:34:GLU:HA	3:C:34:GLU:OE1	2.10	0.50
3:K:42:THR:HG22	3:K:42:THR:O	2.10	0.50
3:G:97:CYS:SG	3:G:98:TYR:N	2.83	0.50
3:K:48:ILE:HG22	3:K:50:ARG:H	1.77	0.50
3:C:130:ILE:HG21	3:C:154:LEU:HD23	1.93	0.50
4:H:145:ASP:OD2	4:H:147:SER:OG	2.29	0.50
3:G:34:GLU:OE2	3:G:34:GLU:HA	2.13	0.49
3:G:252:ILE:HG22	3:G:252:ILE:O	2.11	0.49
3:K:34:GLU:HA	3:K:34:GLU:OE2	2.12	0.49
2:J:48:ILE:HG23	2:J:53:ARG:O	2.12	0.49
3:K:231:ASP:OD1	3:K:231:ASP:N	2.41	0.49
2:B:12:SER:O	2:B:13:LEU:HD22	2.12	0.49
3:C:31:ASN:OD1	3:C:33:GLN:N	2.46	0.49
1:I:87:THR:HG23	1:I:87:THR:O	2.13	0.48
3:G:91:GLU:OE1	3:G:92:ASN:ND2	2.47	0.48
3:K:13:ILE:HG23	3:K:13:ILE:O	2.13	0.48
3:C:97:CYS:SG	3:C:98:TYR:N	2.85	0.48
3:G:198:GLN:OE1	3:G:198:GLN:N	2.43	0.48
3:G:70:LEU:CD1	3:G:112:ILE:HD11	2.44	0.48
4:D:145:ASP:OD2	4:D:147:SER:OG	2.31	0.47
1:I:2:VAL:HG11	1:I:102:TYR:HD2	1.79	0.47
4:D:48:ILE:CD1	4:D:107:THR:HG23	2.45	0.47
1:E:100(K):ASP:N	1:E:100(K):ASP:OD1	2.48	0.47
2:F:100:GLN:HA	2:F:100:GLN:OE1	2.15	0.47
3:G:70:LEU:HD11	3:G:112:ILE:HD11	1.96	0.47
3:G:48:ILE:HG22	3:G:50:ARG:H	1.78	0.47
2:B:100:GLN:HA	2:B:100:GLN:OE1	2.14	0.47
4:D:131:GLU:OE2	4:D:170:ARG:NH1	2.48	0.46
3:C:48:ILE:HG22	3:C:50:ARG:H	1.80	0.46
2:J:100:GLN:HA	2:J:100:GLN:OE1	2.14	0.46
1:A:87:THR:O	1:A:87:THR:HG23	2.15	0.46
2:B:82:ASP:OD1	2:B:82:ASP:C	2.53	0.46
3:G:13:ILE:HG23	3:G:13:ILE:O	2.15	0.46
1:E:84:SER:HA	1:E:111:VAL:HG21	1.96	0.46
3:K:34:GLU:OE1	3:K:321:ARG:HD3	2.16	0.46
4:L:133:ASP:OD1	4:L:133:ASP:C	2.53	0.46
3:C:70:LEU:CD1	3:C:112:ILE:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:LEU:C	2:F:48:ILE:HD13	2.36	0.46
2:F:82:ASP:OD1	2:F:82:ASP:C	2.54	0.46
3:G:48:ILE:HD12	3:G:48:ILE:N	2.31	0.46
3:C:31:ASN:OD1	3:C:34:GLU:N	2.49	0.46
3:C:70:LEU:HD11	3:C:112:ILE:HD11	1.97	0.46
3:K:150:GLU:O	3:K:151:LEU:HD12	2.16	0.46
1:A:100(K):ASP:OD1	1:A:100(K):ASP:N	2.47	0.45
3:C:53:MET:HE3	3:C:88:ILE:HD11	1.98	0.45
2:J:82:ASP:OD2	2:J:82:ASP:C	2.54	0.45
3:K:252:ILE:HG22	3:K:252:ILE:O	2.16	0.45
4:L:4:GLY:O	4:L:5:ALA:HB3	2.17	0.45
3:K:70:LEU:HD11	3:K:112:ILE:HD11	1.99	0.45
3:K:120:LYS:NZ	3:K:150:GLU:OE2	2.47	0.45
3:G:83:MET:CE	3:G:83:MET:N	2.80	0.45
3:C:323:VAL:O	3:C:323:VAL:HG13	2.18	0.44
3:G:61:LEU:HG	3:G:87:LEU:HD11	1.98	0.44
2:B:21:LEU:HD22	2:B:102:THR:HG21	1.99	0.44
3:G:42:THR:O	3:G:42:THR:HG22	2.16	0.44
3:G:150:GLU:O	3:G:151:LEU:HD12	2.18	0.44
3:K:48:ILE:HD12	3:K:48:ILE:N	2.32	0.44
3:K:17:HIS:ND1	3:K:320:MET:HE3	2.33	0.44
3:C:150:GLU:O	3:C:151:LEU:HD12	2.17	0.44
2:F:29:SER:OG	2:F:31:THR:HG22	2.18	0.44
2:F:47:LEU:CD2	2:F:58:ILE:HD11	2.48	0.44
4:D:150:GLU:CD	7:D:301:NAG:H82	2.38	0.44
1:A:100(G):ASP:OD1	1:A:100(L):ARG:NH1	2.51	0.44
4:D:4:GLY:O	4:D:5:ALA:HB3	2.18	0.44
3:G:27:LYS:NZ	3:G:32:GLU:OE1	2.51	0.44
3:K:301:THR:OG1	3:K:305:CYS:SG	2.58	0.43
4:L:158:ASP:OD1	4:L:160:SER:OG	2.34	0.43
6:R:1:NAG:O7	6:R:1:NAG:C3	2.66	0.43
6:R:1:NAG:HO3	6:R:1:NAG:C7	2.16	0.43
3:C:248:ASN:OD1	3:C:248:ASN:C	2.57	0.43
1:E:97:ILE:HG13	1:E:100(L):ARG:HB3	2.01	0.43
4:H:4:GLY:O	4:H:5:ALA:HB3	2.18	0.43
3:K:198:GLN:N	3:K:198:GLN:OE1	2.51	0.43
1:I:100(K):ASP:OD1	1:I:100(K):ASP:N	2.51	0.43
3:K:281:CYS:SG	3:K:282:PHE:N	2.92	0.43
1:A:6:GLN:NE2	1:A:92:CYS:SG	2.92	0.43
3:G:53:MET:CE	3:G:86:THR:HG21	2.48	0.43
2:J:29:SER:OG	2:J:31:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:67:GLU:HB2	4:H:73:ILE:HD11	2.00	0.42
2:B:29:SER:OG	2:B:31:THR:HG22	2.19	0.42
3:G:301:THR:OG1	3:G:305:CYS:SG	2.67	0.42
1:A:70:THR:HG22	1:A:71:SER:N	2.34	0.42
1:E:100(A):ASN:C	1:E:100(C):ASN:H	2.21	0.42
2:F:33:LEU:HD22	2:F:71:PHE:CD1	2.55	0.42
1:I:97:ILE:HD11	1:I:100(L):ARG:HH22	1.82	0.42
3:C:231:ASP:OD1	3:C:231:ASP:N	2.49	0.42
4:L:145:ASP:O	4:L:148:CYS:HB3	2.20	0.42
2:B:49:TYR:CD1	2:B:49:TYR:O	2.73	0.42
3:G:73:THR:HG22	3:G:74:PRO:HD2	2.02	0.42
3:K:97:CYS:SG	3:K:98:TYR:N	2.92	0.42
3:C:281:CYS:SG	3:C:282:PHE:N	2.93	0.42
4:H:6:ILE:HG22	4:H:6:ILE:O	2.20	0.41
3:C:146:SER:OG	3:C:147:PHE:N	2.52	0.41
3:K:291:ARG:HG2	3:K:291:ARG:HH11	1.86	0.41
1:I:28:ILE:HD12	1:I:28:ILE:H	1.86	0.41
1:A:5:VAL:HG12	1:A:6:GLN:N	2.35	0.41
1:E:82(C):LEU:HD23	1:E:84:SER:H	1.86	0.41
3:K:323:VAL:O	3:K:323:VAL:HG13	2.20	0.41
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.02	0.41
2:F:31:THR:HG23	2:F:32:TYR:CD1	2.55	0.41
3:C:53:MET:CE	3:C:88:ILE:HD11	2.50	0.41
3:C:83:MET:N	3:C:83:MET:HE2	2.36	0.41
2:J:47:LEU:HB2	2:J:48:ILE:HD12	2.02	0.41
3:K:70:LEU:CD1	3:K:112:ILE:HD11	2.50	0.41
4:D:48:ILE:HD11	4:D:107:THR:HG23	2.03	0.41
2:F:82:ASP:OD1	2:F:82:ASP:O	2.39	0.41
3:G:64:CYS:HB2	3:G:76:CYS:HB2	1.89	0.41
3:G:137:ARG:HH11	3:G:137:ARG:HG2	1.86	0.40
2:J:82:ASP:OD2	2:J:82:ASP:O	2.40	0.40
4:L:145:ASP:OD1	4:L:145:ASP:N	2.44	0.40
3:K:296:ASN:O	3:K:296:ASN:OD1	2.40	0.40
3:G:83:MET:N	3:G:83:MET:HE2	2.36	0.40
4:H:131:GLU:OE2	4:H:170:ARG:NH1	2.54	0.40
1:I:28:ILE:HD12	1:I:28:ILE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/131 (97%)	119 (94%)	7 (6%)	1 (1%)	16	48
1	E	127/131 (97%)	115 (91%)	11 (9%)	1 (1%)	16	48
1	I	127/131 (97%)	120 (94%)	6 (5%)	1 (1%)	16	48
2	B	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
2	F	106/108 (98%)	100 (94%)	5 (5%)	1 (1%)	14	46
2	J	106/108 (98%)	103 (97%)	3 (3%)	0	100	100
3	C	320/325 (98%)	306 (96%)	14 (4%)	0	100	100
3	G	320/325 (98%)	312 (98%)	8 (2%)	0	100	100
3	K	320/325 (98%)	308 (96%)	12 (4%)	0	100	100
4	D	170/230 (74%)	165 (97%)	5 (3%)	0	100	100
4	H	170/230 (74%)	163 (96%)	6 (4%)	1 (1%)	22	54
4	L	170/230 (74%)	162 (95%)	7 (4%)	1 (1%)	22	54
All	All	2169/2382 (91%)	2077 (96%)	86 (4%)	6 (0%)	38	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	55	ALA
1	A	32	TYR
1	E	32	TYR
1	I	32	TYR
4	H	5	ALA
4	L	5	ALA

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	104/106 (98%)	102 (98%)	2 (2%)	52	69
1	E	104/106 (98%)	100 (96%)	4 (4%)	28	53
1	I	104/106 (98%)	101 (97%)	3 (3%)	37	58
2	B	91/91 (100%)	88 (97%)	3 (3%)	33	56
2	F	91/91 (100%)	90 (99%)	1 (1%)	70	81
2	J	91/91 (100%)	89 (98%)	2 (2%)	47	65
3	C	272/274 (99%)	258 (95%)	14 (5%)	20	46
3	G	272/274 (99%)	264 (97%)	8 (3%)	37	58
3	K	272/274 (99%)	264 (97%)	8 (3%)	37	58
4	D	147/194 (76%)	144 (98%)	3 (2%)	50	68
4	H	147/194 (76%)	144 (98%)	3 (2%)	50	68
4	L	147/194 (76%)	141 (96%)	6 (4%)	26	51
All	All	1842/1995 (92%)	1785 (97%)	57 (3%)	37	57

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	95	ASP
2	B	60	ASP
2	B	65	SER
2	B	82	ASP
3	C	18	HIS
3	C	76	CYS
3	C	83	MET
3	C	139	CYS
3	C	169	ARG
3	C	170	ASN
3	C	191	LYS
3	C	201	SER
3	C	210	ARG
3	C	231	ASP
3	C	271	ASP
3	C	279	SER
3	C	298	SER

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Mol	Chain	Res	Type
3	C	313	SER
4	D	17	MET
4	D	72	GLU
4	D	113	SER
1	E	18	VAL
1	E	50	TRP
1	E	87	THR
1	E	105	GLN
2	F	82	ASP
3	G	18	HIS
3	G	78	LEU
3	G	83	MET
3	G	139	CYS
3	G	210	ARG
3	G	271	ASP
3	G	279	SER
3	G	298	SER
4	H	72	GLU
4	H	113	SER
4	H	148	CYS
1	I	50	TRP
1	I	100(H)	ASP
1	I	100(L)	ARG
2	J	60	ASP
2	J	82	ASP
3	K	76	CYS
3	K	139	CYS
3	K	169	ARG
3	K	231	ASP
3	K	271	ASP
3	K	279	SER
3	K	298	SER
3	K	301	THR
4	L	17	MET
4	L	68	SER
4	L	72	GLU
4	L	110	MET
4	L	133	ASP
4	L	170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	184	HIS
4	D	95	GLN
1	E	105	GLN
3	G	184	HIS
3	G	304	GLN
4	H	125	GLN
3	K	49	ASN
3	K	184	HIS
3	K	296	ASN
3	K	304	GLN
4	L	79	ASN
4	L	125	GLN
4	L	172	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	$\#\|Z\|>2$
5	NAG	M	1	5,3	14,14,15	0.73	0	17,19,21	0.94	0
5	NAG	M	2	5	14,14,15	0.70	0	17,19,21	0.91	0
5	NAG	N	1	5,3	14,14,15	0.71	0	17,19,21	0.81	0
5	NAG	N	2	5	14,14,15	0.71	0	17,19,21	0.83	0
6	NAG	O	1	4,6	14,14,15	0.85	0	17,19,21	1.53	3 (17%)
6	NAG	O	2	6	14,14,15	0.73	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	O	3	6	11,11,12	0.80	0	15,15,17	1.89	2 (13%)
5	NAG	P	1	5,3	14,14,15	0.73	0	17,19,21	0.91	0
5	NAG	P	2	5	14,14,15	0.72	0	17,19,21	0.83	0
5	NAG	Q	1	5,3	14,14,15	0.73	0	17,19,21	0.84	0
5	NAG	Q	2	5	14,14,15	0.70	0	17,19,21	0.82	0
6	NAG	R	1	4,6	14,14,15	0.83	0	17,19,21	1.55	3 (17%)
6	NAG	R	2	6	14,14,15	0.75	0	17,19,21	1.08	1 (5%)
6	BMA	R	3	6	11,11,12	0.80	0	15,15,17	1.89	2 (13%)
5	NAG	S	1	5,3	14,14,15	0.73	0	17,19,21	0.99	0
5	NAG	S	2	5	14,14,15	0.72	0	17,19,21	0.82	0
5	NAG	T	1	5,3	14,14,15	0.72	0	17,19,21	0.83	0
5	NAG	T	2	5	14,14,15	0.71	0	17,19,21	0.82	0
6	NAG	U	1	4,6	14,14,15	0.73	0	17,19,21	1.20	1 (5%)
6	NAG	U	2	6	14,14,15	0.69	0	17,19,21	0.91	1 (5%)
6	BMA	U	3	6	11,11,12	0.80	0	15,15,17	1.93	3 (20%)

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
5	NAG	M	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
6	NAG	O	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	1/2/19/22	0/1/1/1
5	NAG	P	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
6	NAG	R	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	1/2/19/22	0/1/1/1
5	NAG	S	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	NAG	T	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	U	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	U	3	BMA	C1-O5-C5	5.75	119.89	112.19
6	R	3	BMA	C1-O5-C5	5.69	119.81	112.19
6	O	3	BMA	C1-O5-C5	5.66	119.77	112.19
6	O	1	NAG	O5-C1-C2	-3.82	105.38	111.29
6	R	1	NAG	O5-C1-C2	-3.68	105.60	111.29
6	R	1	NAG	C2-N2-C7	2.71	126.53	122.90
6	U	1	NAG	C1-O5-C5	2.64	115.72	112.19
6	O	1	NAG	C2-N2-C7	2.50	126.25	122.90
6	O	2	NAG	O5-C1-C2	-2.38	107.61	111.29
6	R	2	NAG	O5-C1-C2	-2.35	107.66	111.29
6	U	2	NAG	O5-C1-C2	-2.32	107.70	111.29
6	U	3	BMA	C3-C4-C5	2.16	114.15	110.23
6	R	3	BMA	C3-C4-C5	2.12	114.07	110.23
6	O	3	BMA	C3-C4-C5	2.10	114.05	110.23
6	O	1	NAG	C4-C3-C2	2.08	114.07	111.02
6	U	3	BMA	O4-C4-C3	-2.06	105.53	110.38
6	R	1	NAG	C4-C3-C2	2.05	114.02	111.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	1	NAG	C1-C2-N2-C7
6	O	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7
6	U	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
6	U	1	NAG	C3-C2-N2-C7
5	M	2	NAG	C1-C2-N2-C7
5	N	1	NAG	C1-C2-N2-C7
5	Q	1	NAG	C1-C2-N2-C7
5	T	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	M	2	NAG	C3-C2-N2-C7
5	N	1	NAG	C3-C2-N2-C7
5	Q	1	NAG	C3-C2-N2-C7
5	S	1	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7

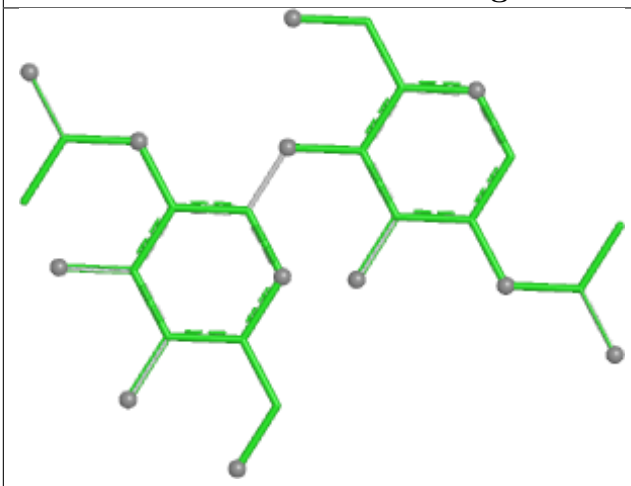
There are no ring outliers.

3 monomers are involved in 5 short contacts:

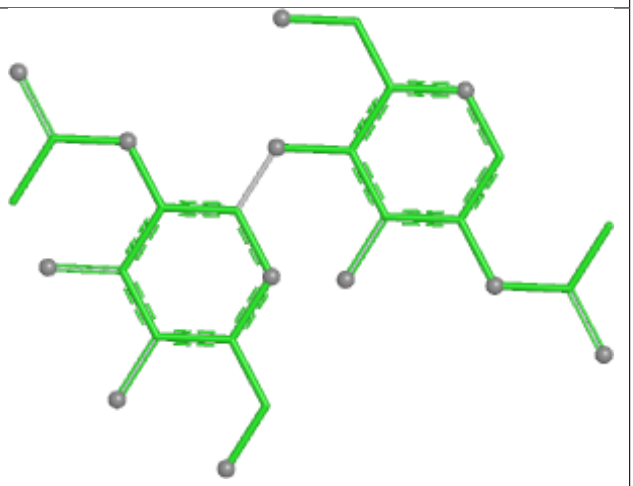
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	1	NAG	1	0
6	R	1	NAG	3	0
5	Q	1	NAG	1	0

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

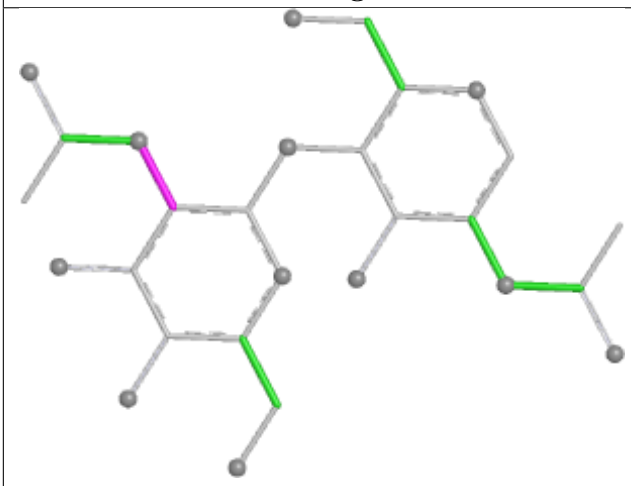
Oligosaccharide Chain M



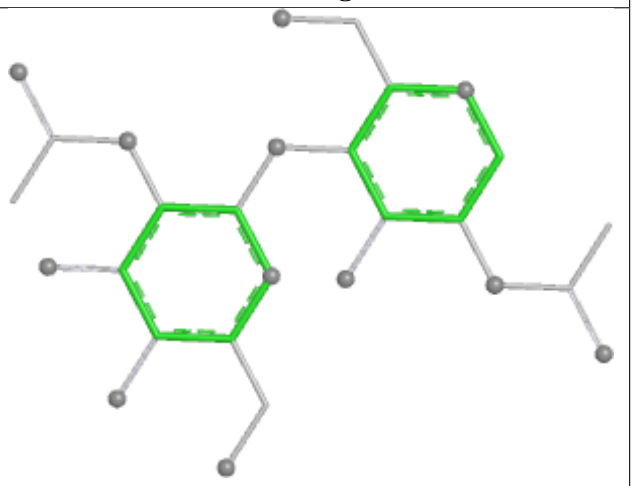
Bond lengths



Bond angles

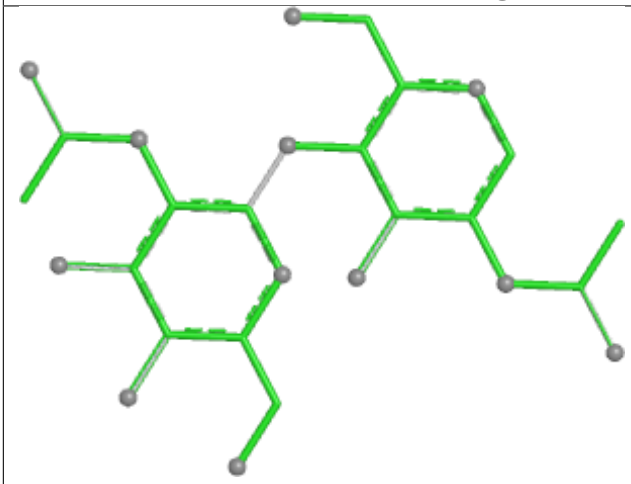


Torsions

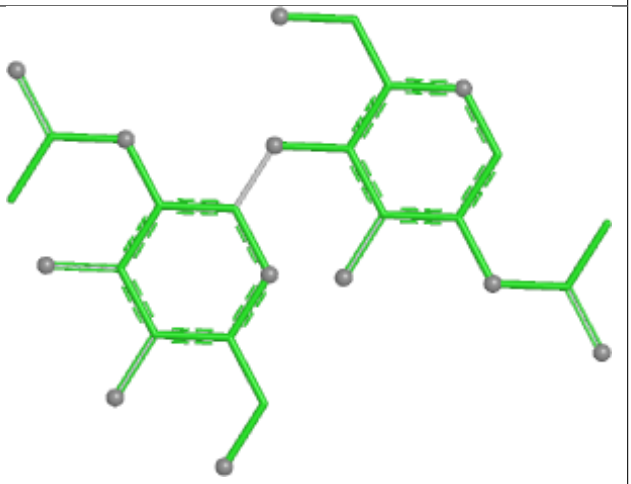


Rings

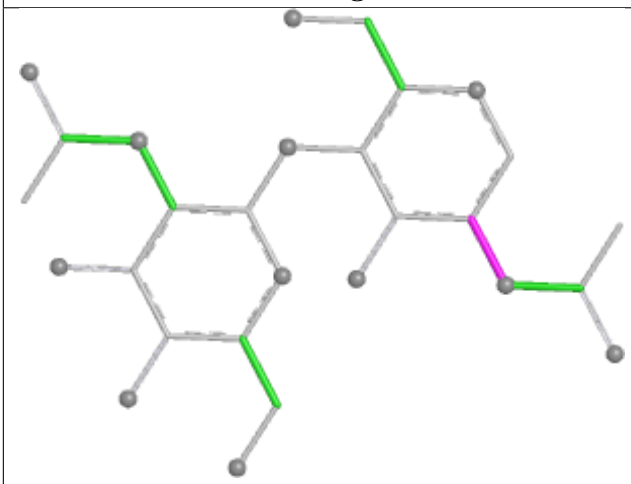
Oligosaccharide Chain N



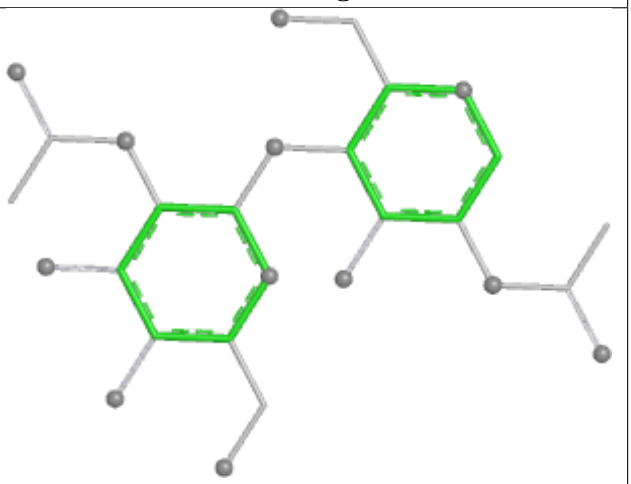
Bond lengths



Bond angles

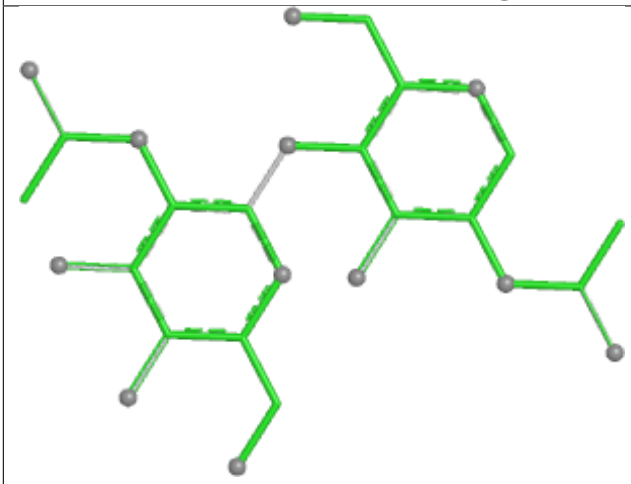


Torsions

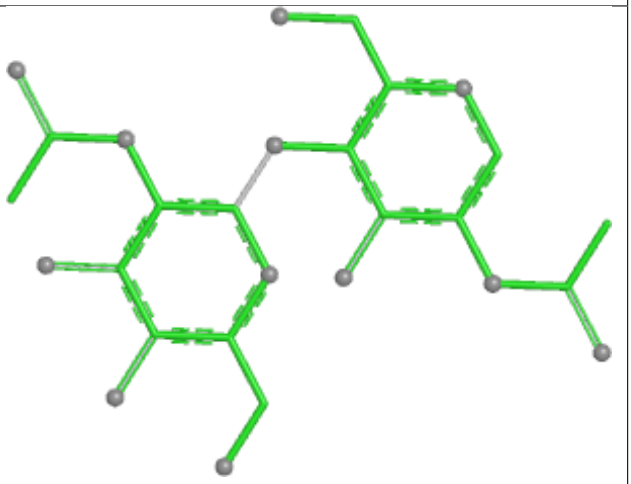


Rings

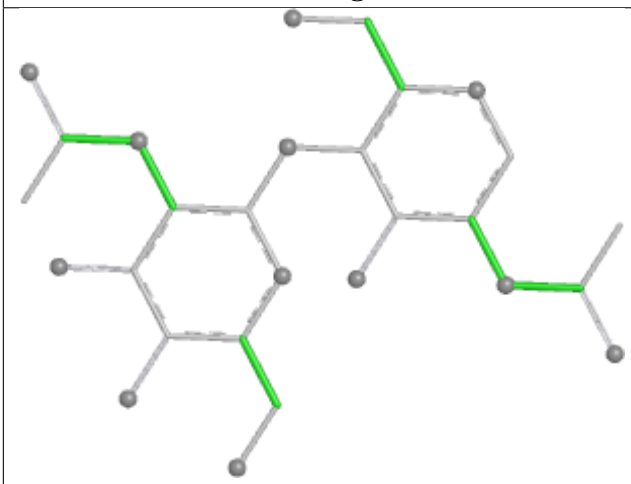
Oligosaccharide Chain P



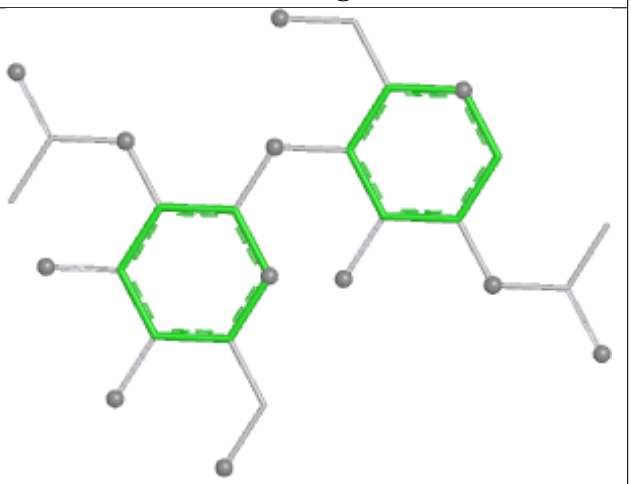
Bond lengths



Bond angles

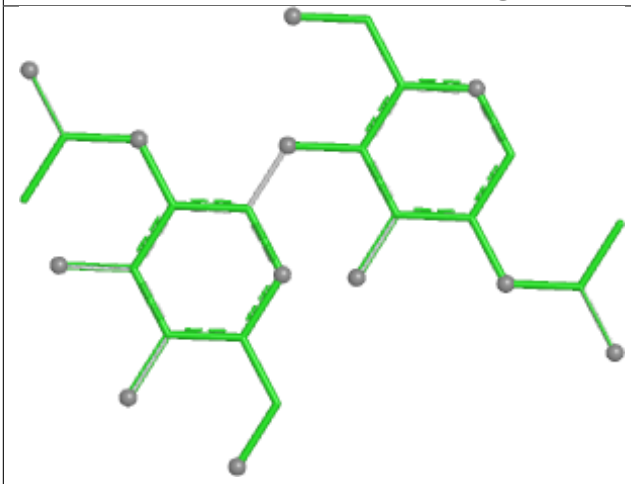


Torsions

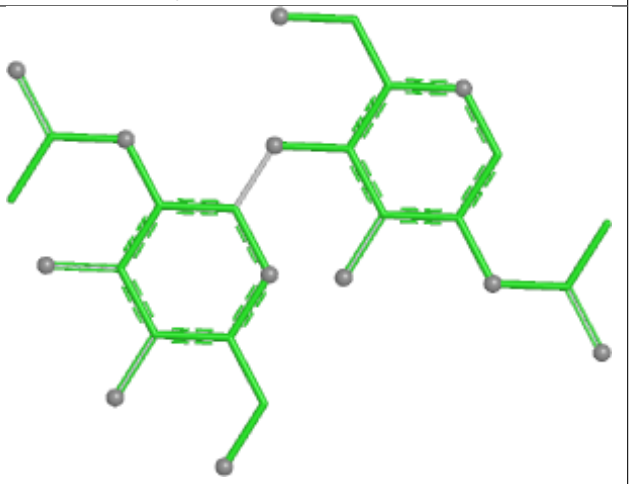


Rings

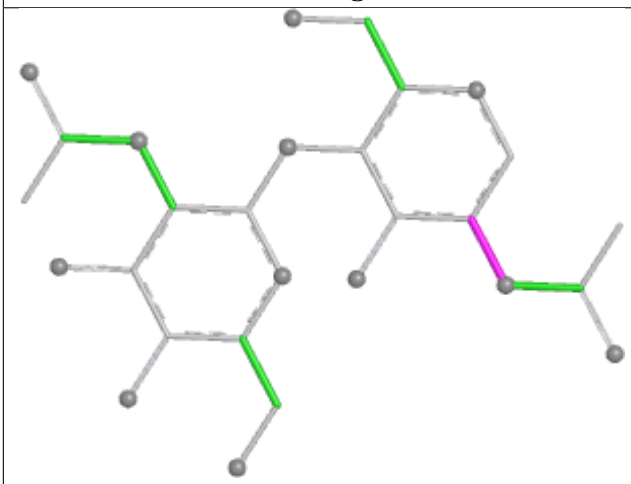
Oligosaccharide Chain Q



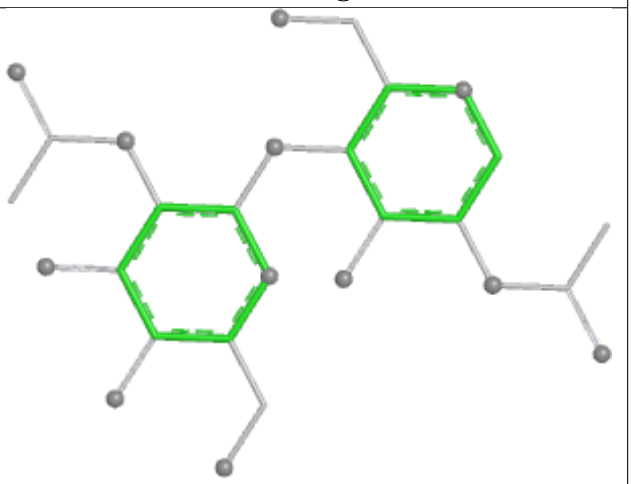
Bond lengths



Bond angles

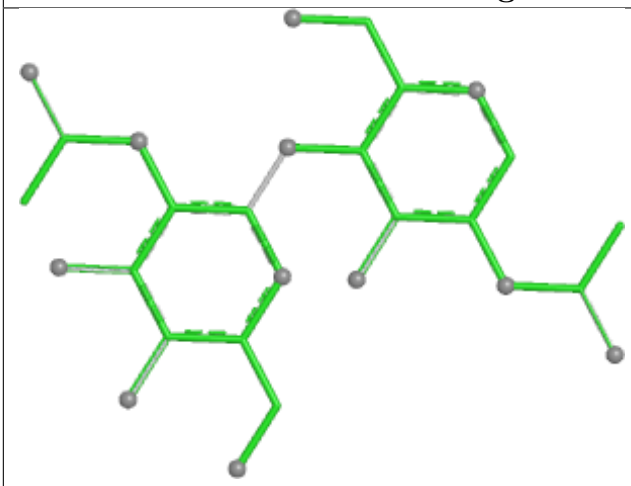


Torsions

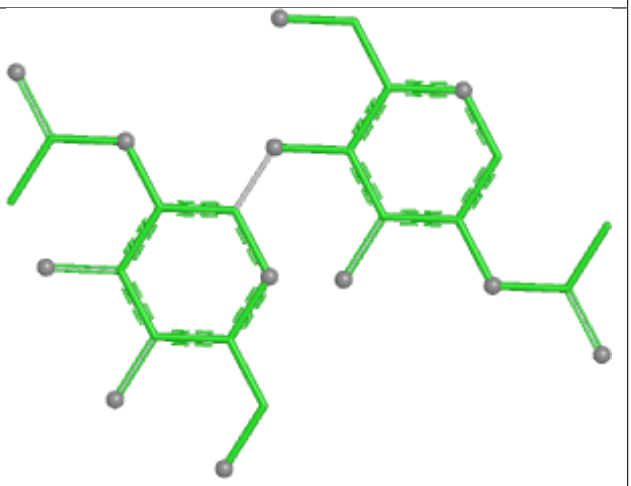


Rings

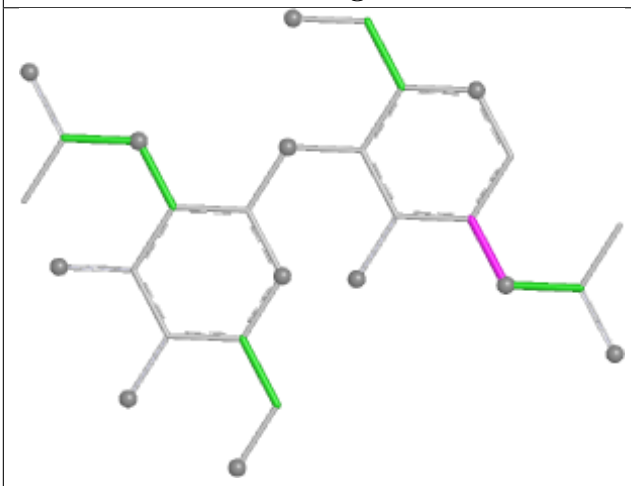
Oligosaccharide Chain S



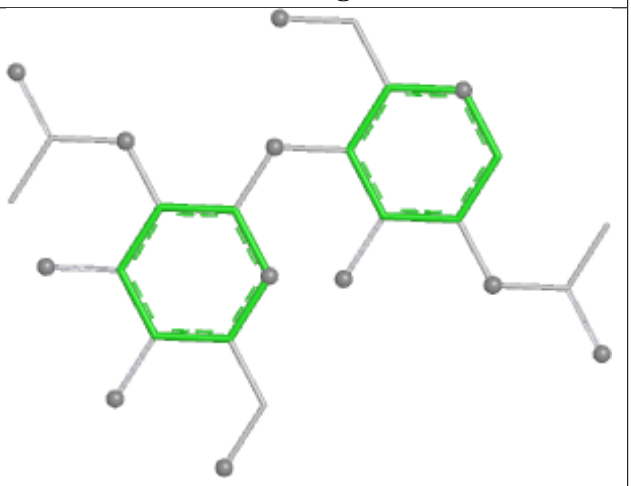
Bond lengths



Bond angles

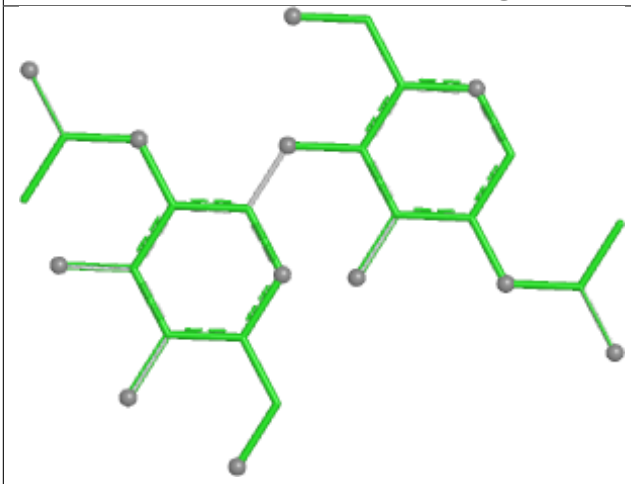


Torsions

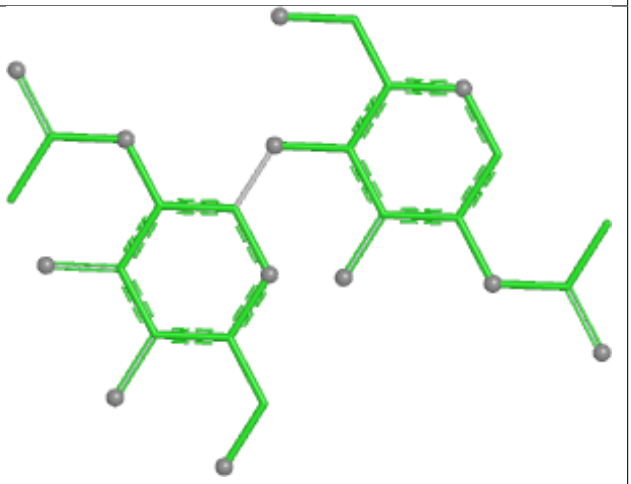


Rings

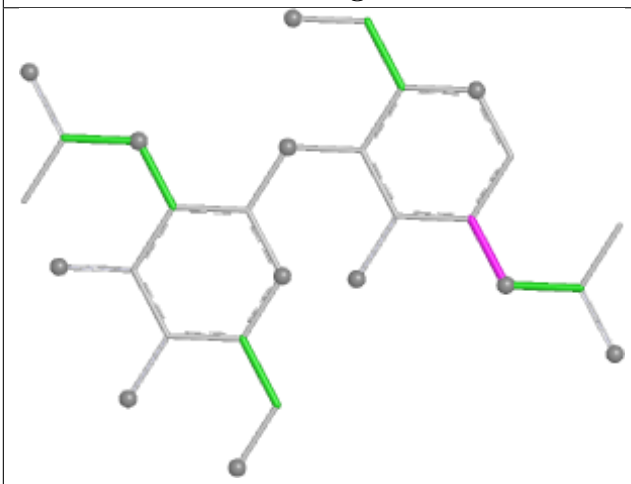
Oligosaccharide Chain T



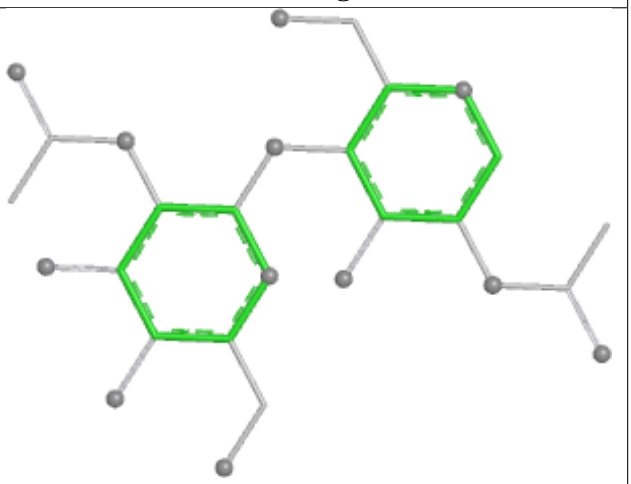
Bond lengths



Bond angles

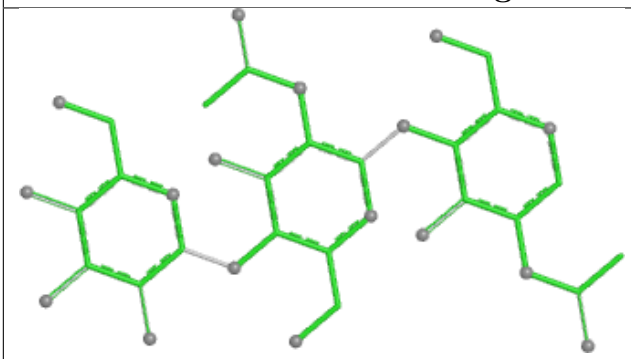


Torsions

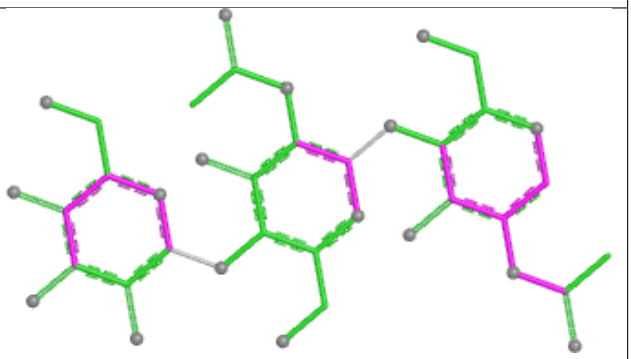


Rings

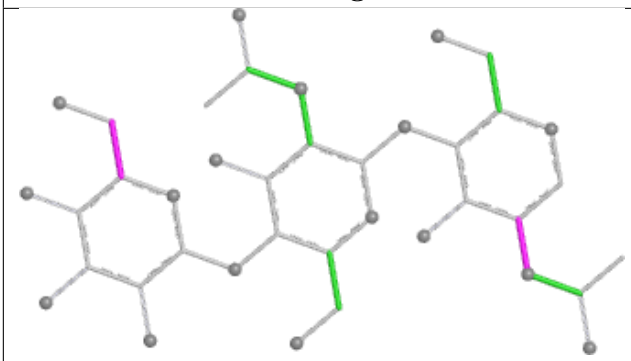
Oligosaccharide Chain O



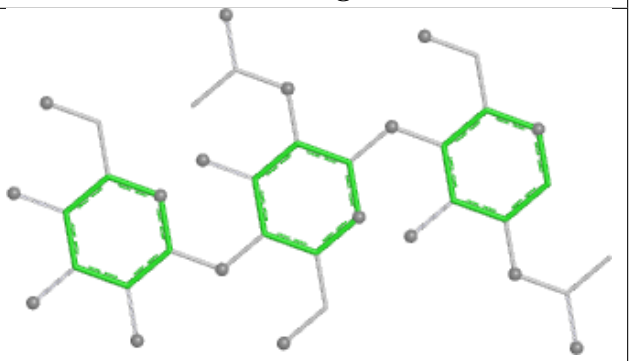
Bond lengths



Bond angles

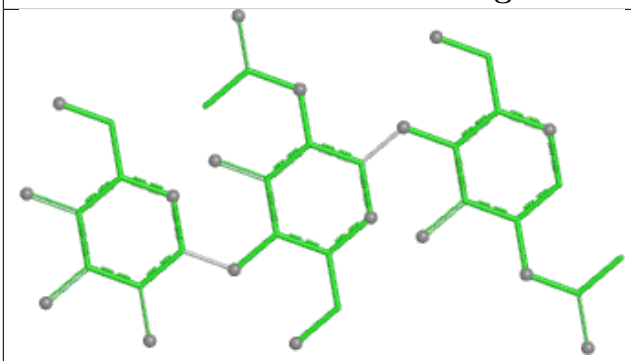


Torsions

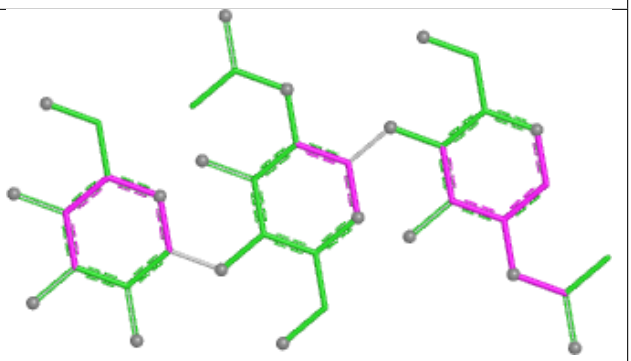


Rings

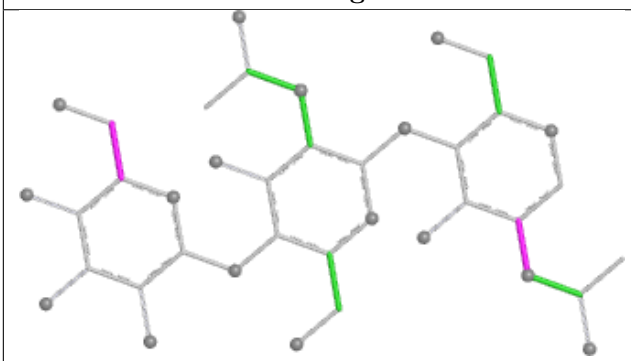
Oligosaccharide Chain R



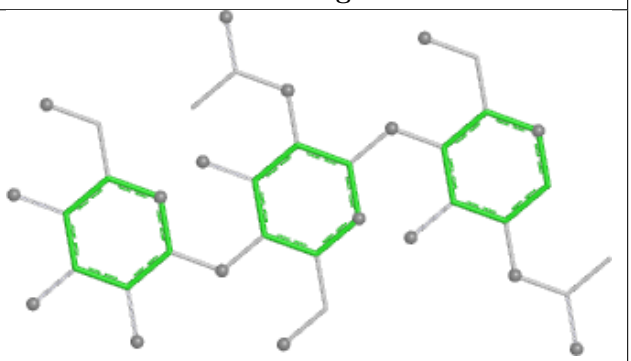
Bond lengths



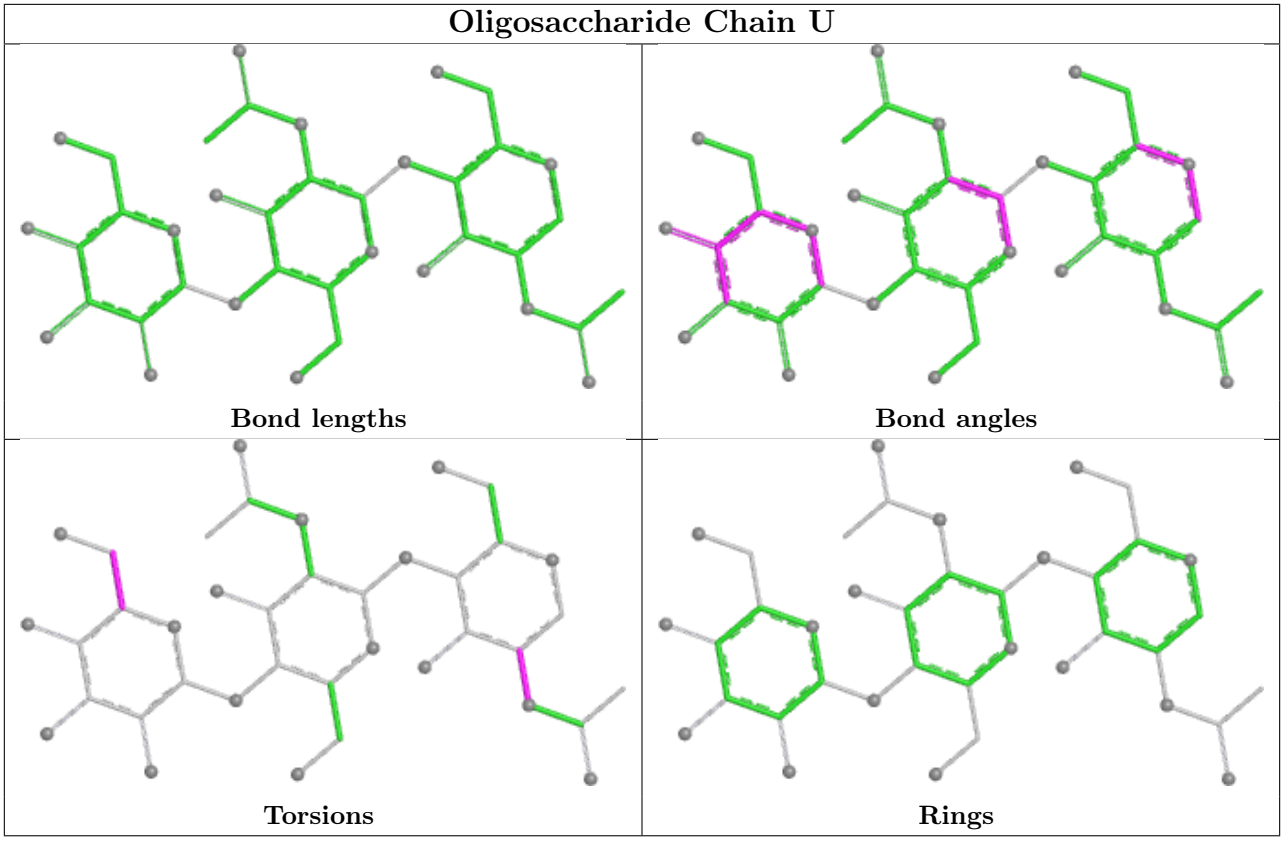
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
7	NAG	L	301	4	14,14,15	0.70	0	17,19,21	0.79	0
7	NAG	H	301	4	14,14,15	0.69	0	17,19,21	0.80	0
7	NAG	D	301	4	14,14,15	0.68	0	17,19,21	0.82	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
7	NAG	L	301	4	-	0/6/23/26	0/1/1/1
7	NAG	H	301	4	-	0/6/23/26	0/1/1/1
7	NAG	D	301	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	301	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.

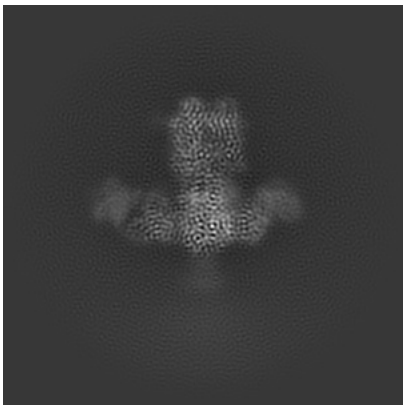
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44901. These allow visual inspection of the internal detail of the map and identification of artifacts.

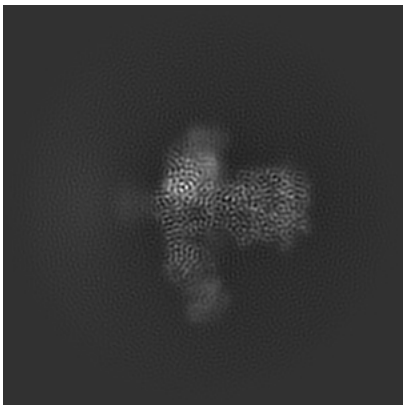
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

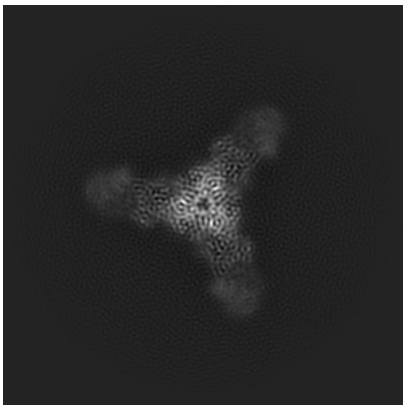
6.1.1 Primary map



X

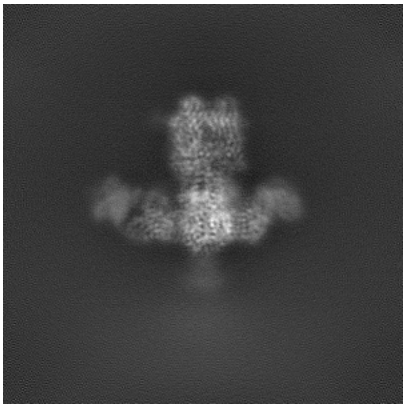


Y

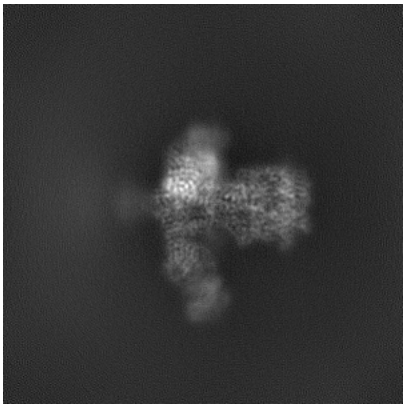


Z

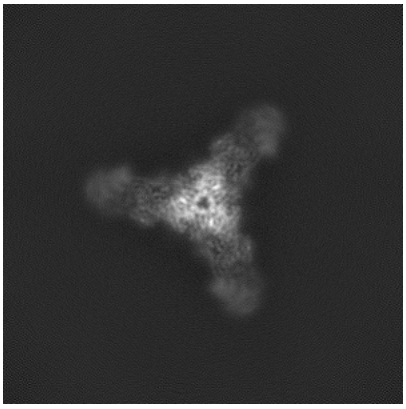
6.1.2 Raw map



X



Y

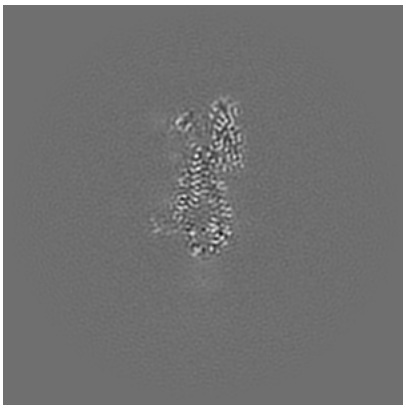


Z

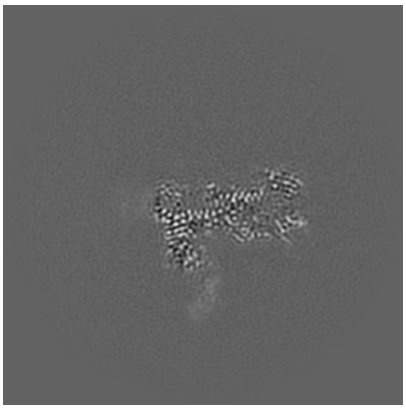
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

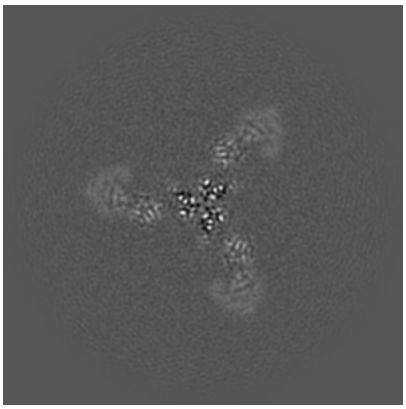
6.2.1 Primary map



X Index: 160

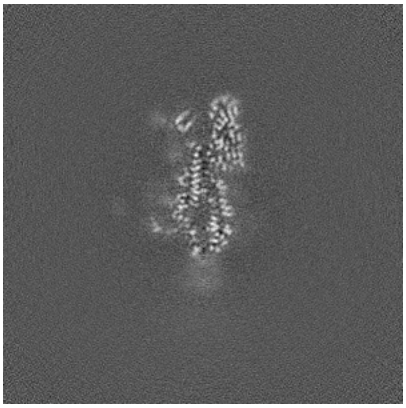


Y Index: 160

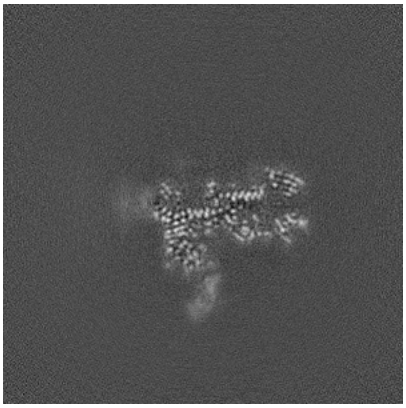


Z Index: 160

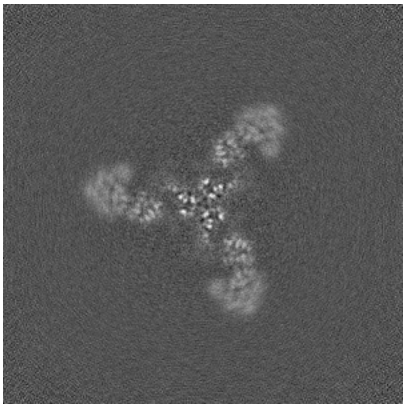
6.2.2 Raw map



X Index: 160



Y Index: 160

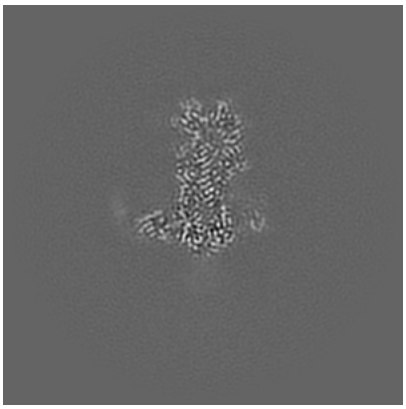


Z Index: 160

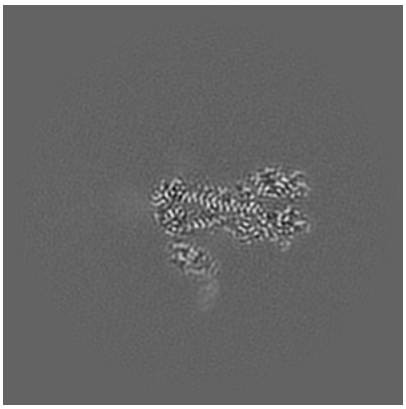
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

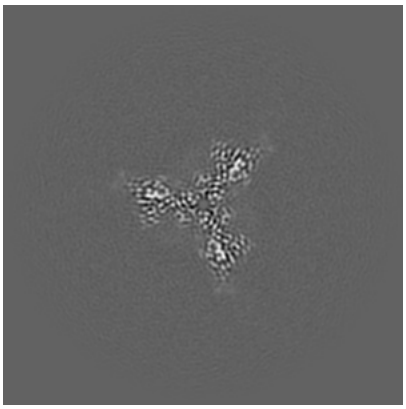
6.3.1 Primary map



X Index: 167

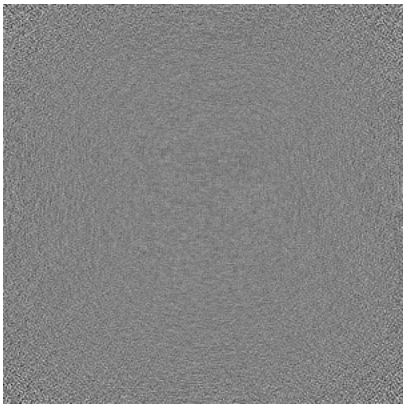


Y Index: 154

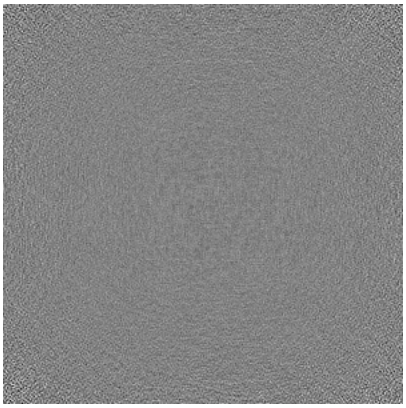


Z Index: 142

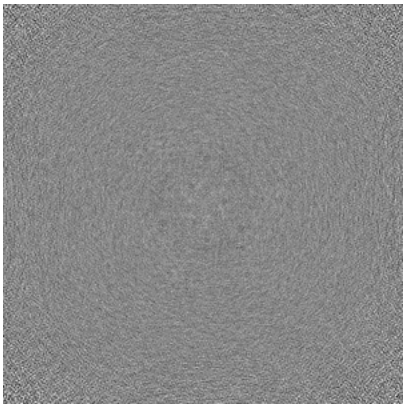
6.3.2 Raw map



X Index: 0



Y Index: 0

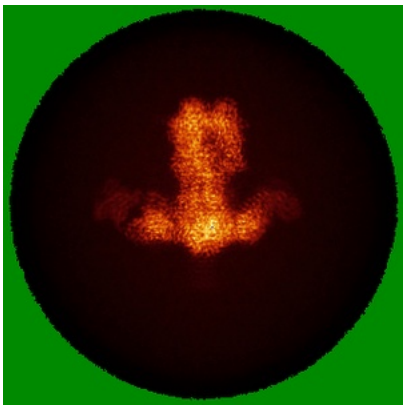


Z Index: 0

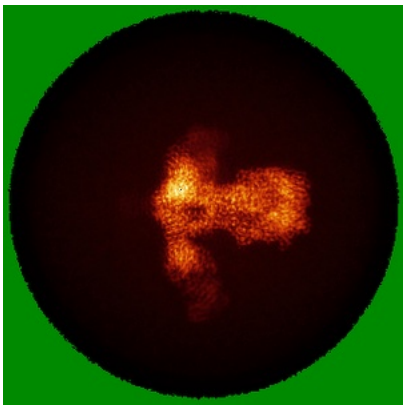
The images above show the largest variance slices of the map in three orthogonal directions.

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

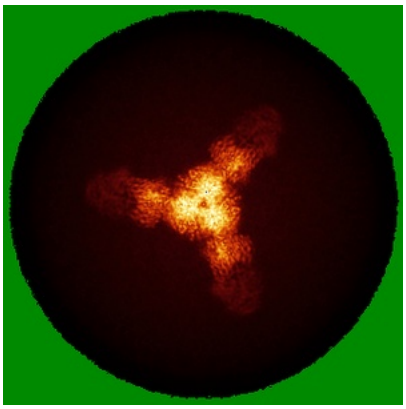
6.4.1 Primary map



X

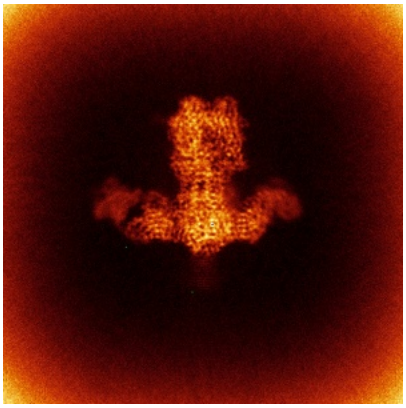


Y

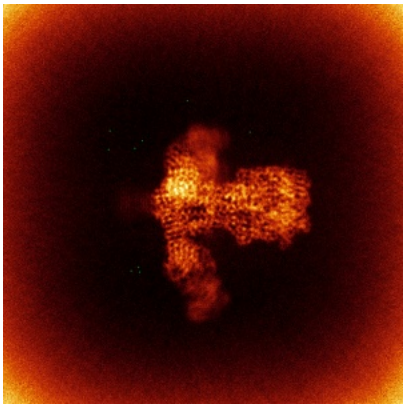


Z

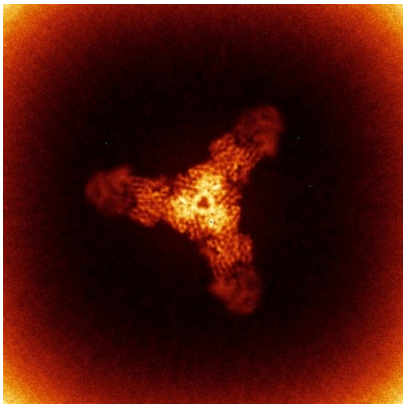
6.4.2 Raw map



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 0.25. 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.

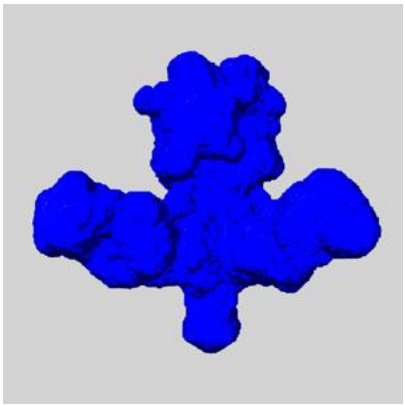
6.6 Mask visualisation

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

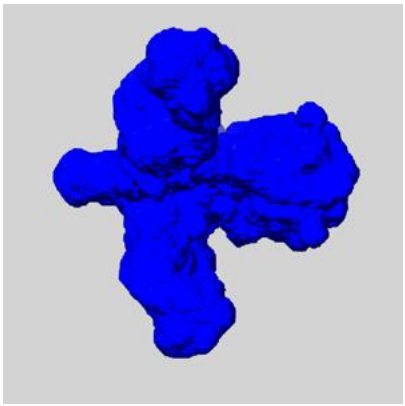
A mask typically either:

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

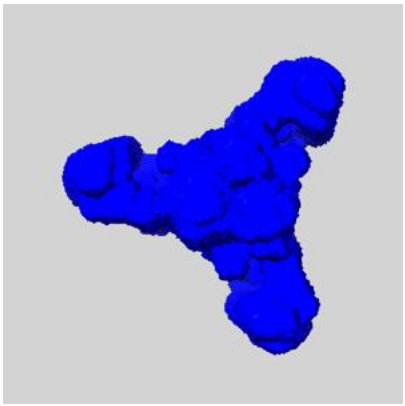
6.6.1 emd_44901_msk_1.map



X



Y

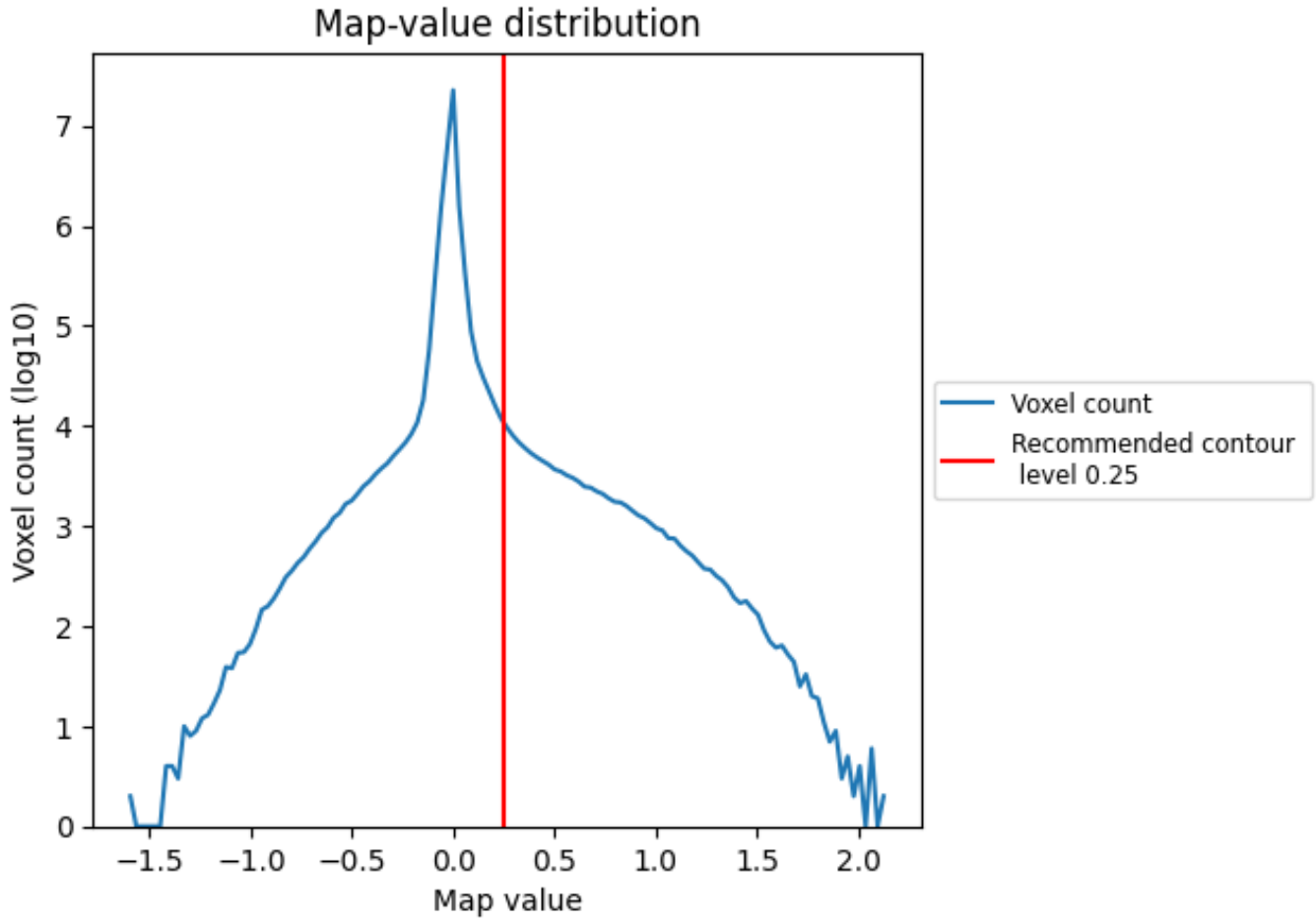


Z

7 Map analysis

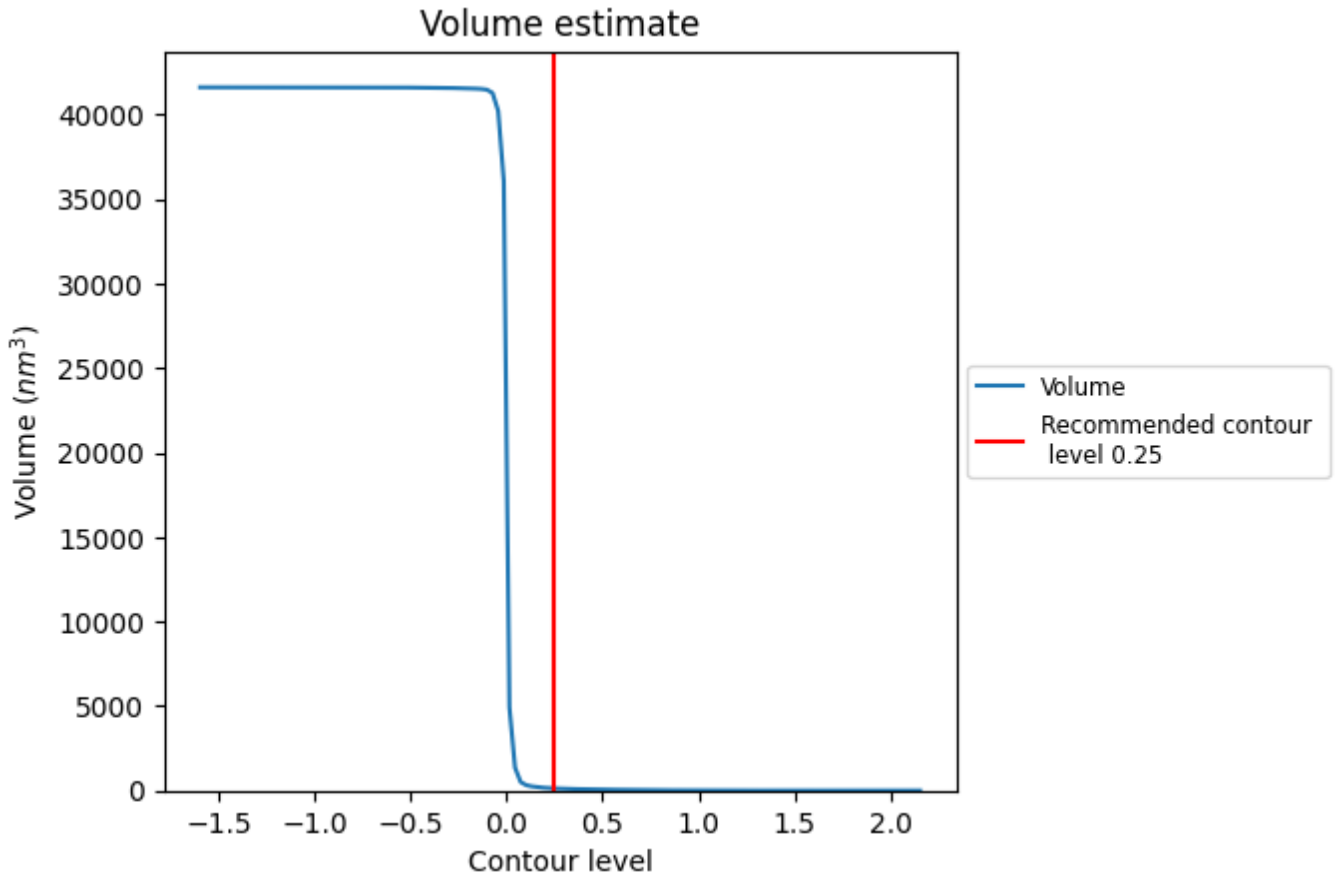
This section contains the results of statistical analysis of the map.

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.

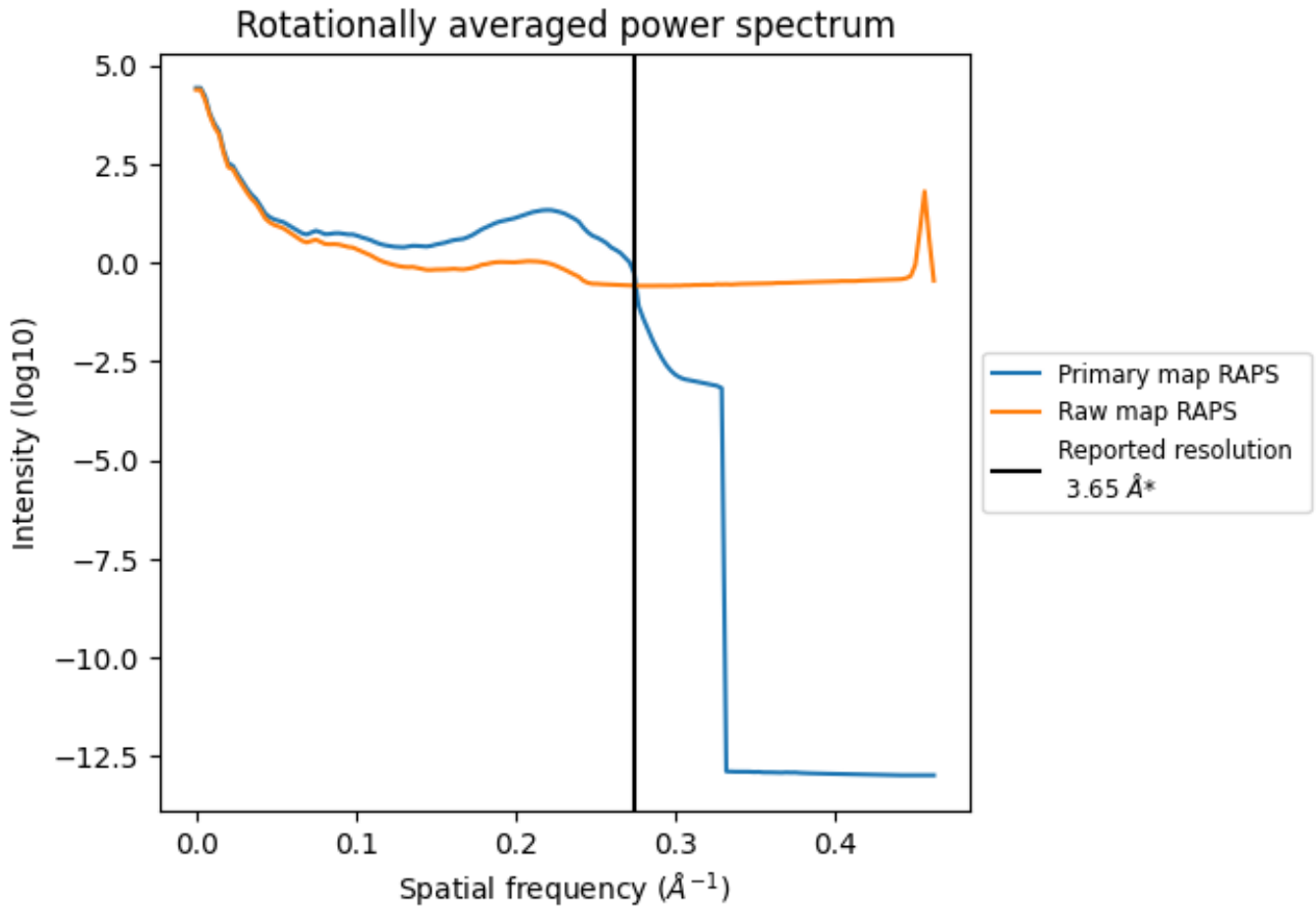
7.2 Volume estimate



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 116 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)

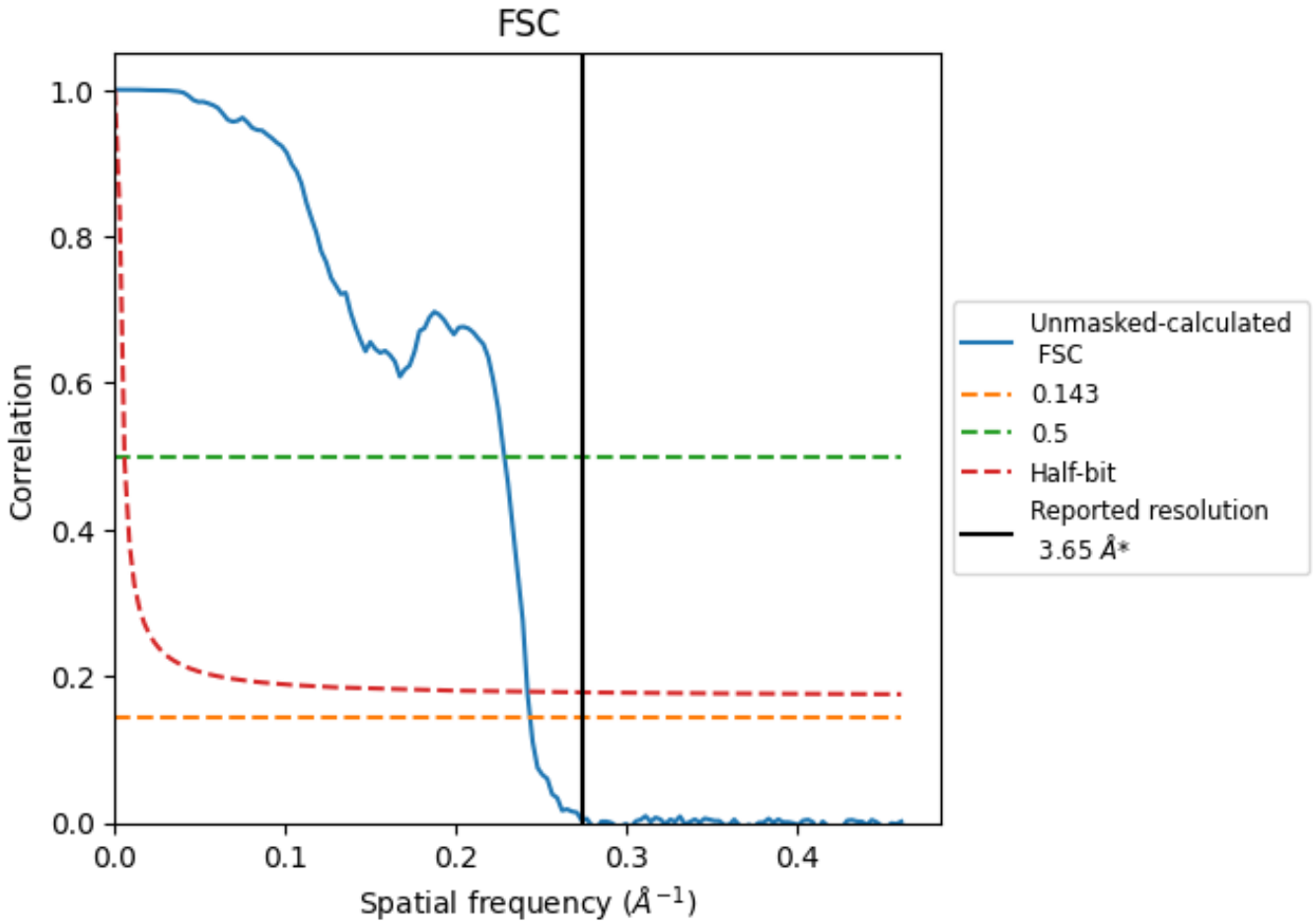


*Reported resolution corresponds to spatial frequency of 0.274 $Å^{-1}$

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 0.274 Å^{-1}

8.2 Resolution estimates (i)

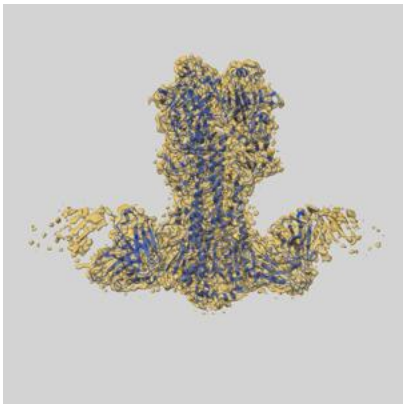
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	4.37	4.13

*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 4.10 differs from the reported value 3.65 by more than 10 %

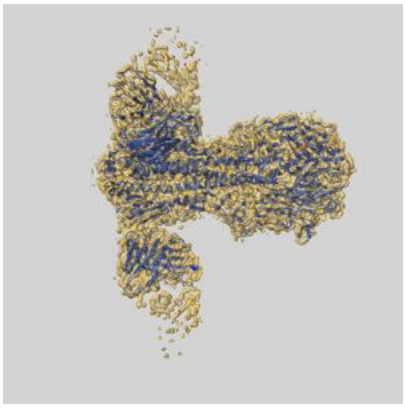
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44901 and PDB model 9BU6. Per-residue inclusion information can be found in section 3 on page 11.

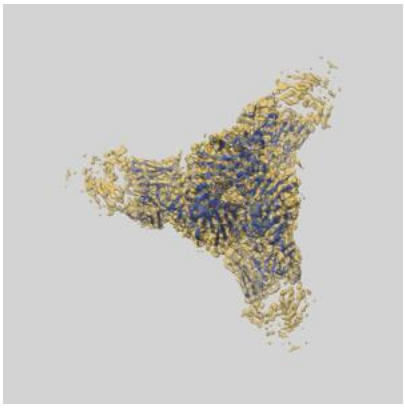
9.1 Map-model overlay



X



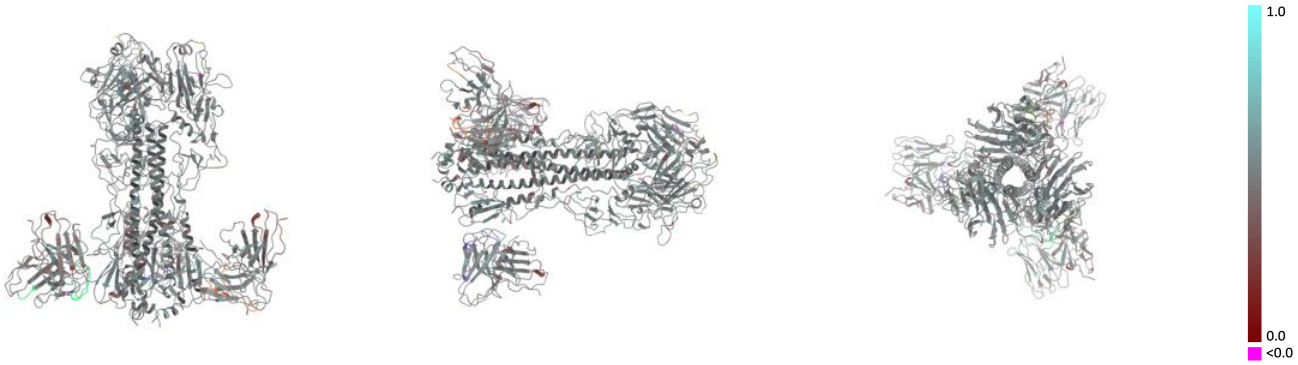
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

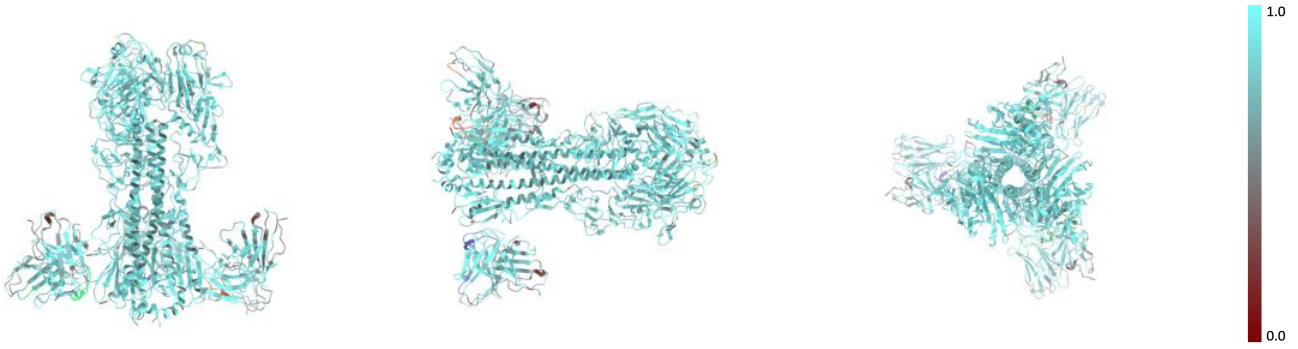
9.2 Q-score mapped to coordinate model (i)



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.

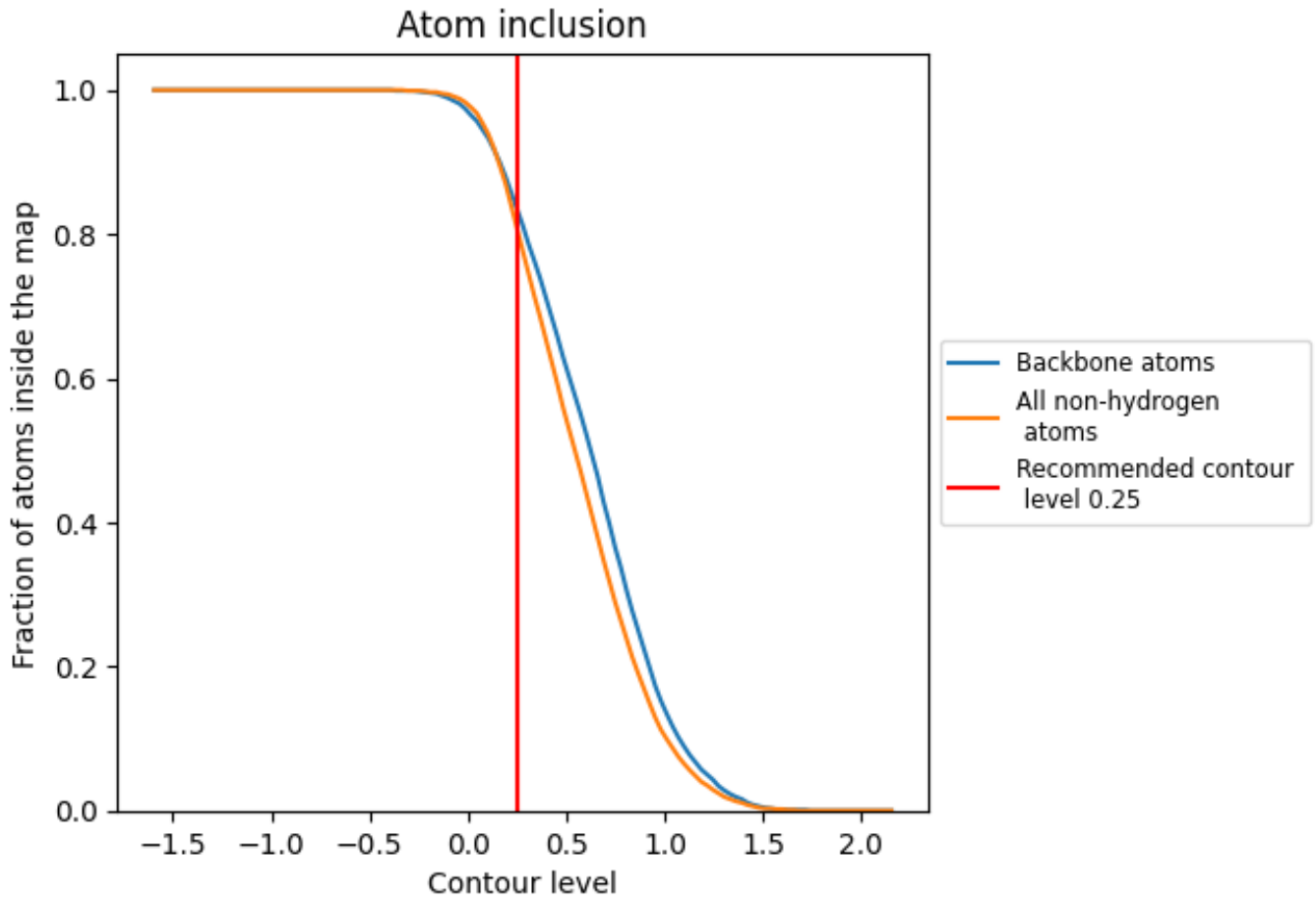
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.4890
A	0.8090	0.4920
B	0.7330	0.4510
C	0.8410	0.4980
D	0.8260	0.4990
E	0.8140	0.4920
F	0.7220	0.4500
G	0.8400	0.5000
H	0.8240	0.4940
I	0.8040	0.4890
J	0.7210	0.4470
K	0.8350	0.5000
L	0.8210	0.4990
M	0.5360	0.3910
N	0.3570	0.4060
O	0.5130	0.3960
P	0.6070	0.4030
Q	0.3570	0.4260
R	0.4870	0.3880
S	0.4640	0.4320
T	0.3570	0.4000
U	0.5640	0.4410