Full wwPDB EM Validation Report (i)

Apr 17, 2025 – 01:26 PM EDT

PDB ID	:	9O8Q / pdb_00009o8q
EMDB ID	:	EMD-70233
Title	:	Cryo-EM structure of NI06063_d30_103 Fab in complex with influenza virus hemagglutinin from A/Hong Kong/485197/2014 (H3N2)
Deposited on	:	2025-04-16
Resolution	:	2.62 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (1)) were used in the production of this report:

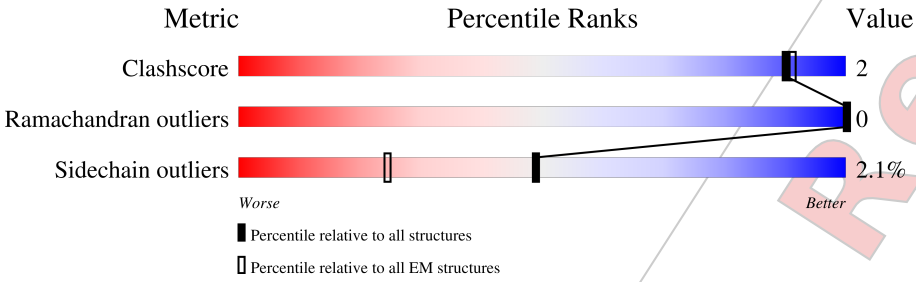
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.62 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	G	121	95% 5%
1	H	121	95% 5%
1	I	121	95% 5%
2	J	109	92% 6% •
2	K	109	94% 5% •
2	L	109	94% 5% •
3	A	345	83% 7% • 8%

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Mol	Chain	Length	Quality of chain
3	C	345	83% 8% 8%
3	D	345	83% 7% 8%
4	B	236	69% 27%
4	E	236	69% 27%
4	F	236	69% 27%
5	M	3	67% 67% 33%
5	O	3	33% 33% 67%
5	P	3	33% 67%
5	Q	3	67% 67% 33%
5	S	3	33% 33% 67%
5	T	3	33% 67%
5	U	3	67% 67% 33%
5	W	3	33% 33% 67%
5	X	3	33% 67%
6	N	3	33% 67%
6	R	3	33% 33% 67%
6	V	3	33% 33% 67%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17502 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 NI06063_d30_103 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	121	Total	C	N	O	S	0	0
			951	605	163	178	5		
1	G	121	Total	C	N	O	S	0	0
			951	605	163	178	5		
1	I	121	Total	C	N	O	S	0	0
			951	605	163	178	5		

- Molecule 2 is a protein called NI06063_d30_103 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total	C	N	O	S	0	0
			771	477	134	156	4		
2	J	107	Total	C	N	O	S	0	0
			771	477	134	156	4		
2	K	107	Total	C	N	O	S	0	0
			771	477	134	156	4		

- Molecule 3 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	316	Total	C	N	O	S	0	0
			2471	1549	439	471	12		
3	C	316	Total	C	N	O	S	0	0
			2471	1549	439	471	12		
3	D	316	Total	C	N	O	S	0	0
			2471	1549	439	471	12		

- Molecule 4 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	172	Total	C	N	O	S	0	0
			1388	863	246	273	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	172	Total	C	N	O	S	0	0
			1388	863	246	273	6		
4	F	172	Total	C	N	O	S	0	0
			1388	863	246	273	6		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLY	-	expression tag	UNP A0A0K0YAS1
B	178	TYR	-	expression tag	UNP A0A0K0YAS1
B	179	ILE	-	expression tag	UNP A0A0K0YAS1
B	180	PRO	-	expression tag	UNP A0A0K0YAS1
B	181	GLU	-	expression tag	UNP A0A0K0YAS1
B	182	ALA	-	expression tag	UNP A0A0K0YAS1
B	183	PRO	-	expression tag	UNP A0A0K0YAS1
B	184	ARG	-	expression tag	UNP A0A0K0YAS1
B	185	ASP	-	expression tag	UNP A0A0K0YAS1
B	186	GLY	-	expression tag	UNP A0A0K0YAS1
B	187	GLN	-	expression tag	UNP A0A0K0YAS1
B	188	ALA	-	expression tag	UNP A0A0K0YAS1
B	189	TYR	-	expression tag	UNP A0A0K0YAS1
B	190	VAL	-	expression tag	UNP A0A0K0YAS1
B	191	ARG	-	expression tag	UNP A0A0K0YAS1
B	192	LYS	-	expression tag	UNP A0A0K0YAS1
B	193	ASP	-	expression tag	UNP A0A0K0YAS1
B	194	GLY	-	expression tag	UNP A0A0K0YAS1
B	195	GLU	-	expression tag	UNP A0A0K0YAS1
B	196	TRP	-	expression tag	UNP A0A0K0YAS1
B	197	VAL	-	expression tag	UNP A0A0K0YAS1
B	198	LEU	-	expression tag	UNP A0A0K0YAS1
B	199	LEU	-	expression tag	UNP A0A0K0YAS1
B	200	SER	-	expression tag	UNP A0A0K0YAS1
B	201	THR	-	expression tag	UNP A0A0K0YAS1
B	202	PHE	-	expression tag	UNP A0A0K0YAS1
B	203	LEU	-	expression tag	UNP A0A0K0YAS1
B	204	GLY	-	expression tag	UNP A0A0K0YAS1
B	205	SER	-	expression tag	UNP A0A0K0YAS1
B	206	GLU	-	expression tag	UNP A0A0K0YAS1
B	207	ASN	-	expression tag	UNP A0A0K0YAS1
B	208	LEU	-	expression tag	UNP A0A0K0YAS1
B	209	TYR	-	expression tag	UNP A0A0K0YAS1
B	210	PHE	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	211	GLN	-	expression tag	UNP A0A0K0YAS1
B	212	GLY	-	expression tag	UNP A0A0K0YAS1
B	213	SER	-	expression tag	UNP A0A0K0YAS1
B	214	ALA	-	expression tag	UNP A0A0K0YAS1
B	215	TRP	-	expression tag	UNP A0A0K0YAS1
B	216	SER	-	expression tag	UNP A0A0K0YAS1
B	217	HIS	-	expression tag	UNP A0A0K0YAS1
B	218	PRO	-	expression tag	UNP A0A0K0YAS1
B	219	GLN	-	expression tag	UNP A0A0K0YAS1
B	220	PHE	-	expression tag	UNP A0A0K0YAS1
B	221	GLU	-	expression tag	UNP A0A0K0YAS1
B	222	LYS	-	expression tag	UNP A0A0K0YAS1
B	223	GLY	-	expression tag	UNP A0A0K0YAS1
B	224	GLY	-	expression tag	UNP A0A0K0YAS1
B	225	GLY	-	expression tag	UNP A0A0K0YAS1
B	226	SER	-	expression tag	UNP A0A0K0YAS1
B	227	GLY	-	expression tag	UNP A0A0K0YAS1
B	228	GLY	-	expression tag	UNP A0A0K0YAS1
B	229	GLY	-	expression tag	UNP A0A0K0YAS1
B	230	SER	-	expression tag	UNP A0A0K0YAS1
B	231	HIS	-	expression tag	UNP A0A0K0YAS1
B	232	HIS	-	expression tag	UNP A0A0K0YAS1
B	233	HIS	-	expression tag	UNP A0A0K0YAS1
B	234	HIS	-	expression tag	UNP A0A0K0YAS1
B	235	HIS	-	expression tag	UNP A0A0K0YAS1
B	236	HIS	-	expression tag	UNP A0A0K0YAS1
E	177	GLY	-	expression tag	UNP A0A0K0YAS1
E	178	TYR	-	expression tag	UNP A0A0K0YAS1
E	179	ILE	-	expression tag	UNP A0A0K0YAS1
E	180	PRO	-	expression tag	UNP A0A0K0YAS1
E	181	GLU	-	expression tag	UNP A0A0K0YAS1
E	182	ALA	-	expression tag	UNP A0A0K0YAS1
E	183	PRO	-	expression tag	UNP A0A0K0YAS1
E	184	ARG	-	expression tag	UNP A0A0K0YAS1
E	185	ASP	-	expression tag	UNP A0A0K0YAS1
E	186	GLY	-	expression tag	UNP A0A0K0YAS1
E	187	GLN	-	expression tag	UNP A0A0K0YAS1
E	188	ALA	-	expression tag	UNP A0A0K0YAS1
E	189	TYR	-	expression tag	UNP A0A0K0YAS1
E	190	VAL	-	expression tag	UNP A0A0K0YAS1
E	191	ARG	-	expression tag	UNP A0A0K0YAS1
E	192	LYS	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	193	ASP	-	expression tag	UNP A0A0K0YAS1
E	194	GLY	-	expression tag	UNP A0A0K0YAS1
E	195	GLU	-	expression tag	UNP A0A0K0YAS1
E	196	TRP	-	expression tag	UNP A0A0K0YAS1
E	197	VAL	-	expression tag	UNP A0A0K0YAS1
E	198	LEU	-	expression tag	UNP A0A0K0YAS1
E	199	LEU	-	expression tag	UNP A0A0K0YAS1
E	200	SER	-	expression tag	UNP A0A0K0YAS1
E	201	THR	-	expression tag	UNP A0A0K0YAS1
E	202	PHE	-	expression tag	UNP A0A0K0YAS1
E	203	LEU	-	expression tag	UNP A0A0K0YAS1
E	204	GLY	-	expression tag	UNP A0A0K0YAS1
E	205	SER	-	expression tag	UNP A0A0K0YAS1
E	206	GLU	-	expression tag	UNP A0A0K0YAS1
E	207	ASN	-	expression tag	UNP A0A0K0YAS1
E	208	LEU	-	expression tag	UNP A0A0K0YAS1
E	209	TYR	-	expression tag	UNP A0A0K0YAS1
E	210	PHE	-	expression tag	UNP A0A0K0YAS1
E	211	GLN	-	expression tag	UNP A0A0K0YAS1
E	212	GLY	-	expression tag	UNP A0A0K0YAS1
E	213	SER	-	expression tag	UNP A0A0K0YAS1
E	214	ALA	-	expression tag	UNP A0A0K0YAS1
E	215	TRP	-	expression tag	UNP A0A0K0YAS1
E	216	SER	-	expression tag	UNP A0A0K0YAS1
E	217	HIS	-	expression tag	UNP A0A0K0YAS1
E	218	PRO	-	expression tag	UNP A0A0K0YAS1
E	219	GLN	-	expression tag	UNP A0A0K0YAS1
E	220	PHE	-	expression tag	UNP A0A0K0YAS1
E	221	GLU	-	expression tag	UNP A0A0K0YAS1
E	222	LYS	-	expression tag	UNP A0A0K0YAS1
E	223	GLY	-	expression tag	UNP A0A0K0YAS1
E	224	GLY	-	expression tag	UNP A0A0K0YAS1
E	225	GLY	-	expression tag	UNP A0A0K0YAS1
E	226	SER	-	expression tag	UNP A0A0K0YAS1
E	227	GLY	-	expression tag	UNP A0A0K0YAS1
E	228	GLY	-	expression tag	UNP A0A0K0YAS1
E	229	GLY	-	expression tag	UNP A0A0K0YAS1
E	230	SER	-	expression tag	UNP A0A0K0YAS1
E	231	HIS	-	expression tag	UNP A0A0K0YAS1
E	232	HIS	-	expression tag	UNP A0A0K0YAS1
E	233	HIS	-	expression tag	UNP A0A0K0YAS1
E	234	HIS	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	235	HIS	-	expression tag	UNP A0A0K0YAS1
E	236	HIS	-	expression tag	UNP A0A0K0YAS1
F	177	GLY	-	expression tag	UNP A0A0K0YAS1
F	178	TYR	-	expression tag	UNP A0A0K0YAS1
F	179	ILE	-	expression tag	UNP A0A0K0YAS1
F	180	PRO	-	expression tag	UNP A0A0K0YAS1
F	181	GLU	-	expression tag	UNP A0A0K0YAS1
F	182	ALA	-	expression tag	UNP A0A0K0YAS1
F	183	PRO	-	expression tag	UNP A0A0K0YAS1
F	184	ARG	-	expression tag	UNP A0A0K0YAS1
F	185	ASP	-	expression tag	UNP A0A0K0YAS1
F	186	GLY	-	expression tag	UNP A0A0K0YAS1
F	187	GLN	-	expression tag	UNP A0A0K0YAS1
F	188	ALA	-	expression tag	UNP A0A0K0YAS1
F	189	TYR	-	expression tag	UNP A0A0K0YAS1
F	190	VAL	-	expression tag	UNP A0A0K0YAS1
F	191	ARG	-	expression tag	UNP A0A0K0YAS1
F	192	LYS	-	expression tag	UNP A0A0K0YAS1
F	193	ASP	-	expression tag	UNP A0A0K0YAS1
F	194	GLY	-	expression tag	UNP A0A0K0YAS1
F	195	GLU	-	expression tag	UNP A0A0K0YAS1
F	196	TRP	-	expression tag	UNP A0A0K0YAS1
F	197	VAL	-	expression tag	UNP A0A0K0YAS1
F	198	LEU	-	expression tag	UNP A0A0K0YAS1
F	199	LEU	-	expression tag	UNP A0A0K0YAS1
F	200	SER	-	expression tag	UNP A0A0K0YAS1
F	201	THR	-	expression tag	UNP A0A0K0YAS1
F	202	PHE	-	expression tag	UNP A0A0K0YAS1
F	203	LEU	-	expression tag	UNP A0A0K0YAS1
F	204	GLY	-	expression tag	UNP A0A0K0YAS1
F	205	SER	-	expression tag	UNP A0A0K0YAS1
F	206	GLU	-	expression tag	UNP A0A0K0YAS1
F	207	ASN	-	expression tag	UNP A0A0K0YAS1
F	208	LEU	-	expression tag	UNP A0A0K0YAS1
F	209	TYR	-	expression tag	UNP A0A0K0YAS1
F	210	PHE	-	expression tag	UNP A0A0K0YAS1
F	211	GLN	-	expression tag	UNP A0A0K0YAS1
F	212	GLY	-	expression tag	UNP A0A0K0YAS1
F	213	SER	-	expression tag	UNP A0A0K0YAS1
F	214	ALA	-	expression tag	UNP A0A0K0YAS1
F	215	TRP	-	expression tag	UNP A0A0K0YAS1
F	216	SER	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	217	HIS	-	expression tag	UNP A0A0K0YAS1
F	218	PRO	-	expression tag	UNP A0A0K0YAS1
F	219	GLN	-	expression tag	UNP A0A0K0YAS1
F	220	PHE	-	expression tag	UNP A0A0K0YAS1
F	221	GLU	-	expression tag	UNP A0A0K0YAS1
F	222	LYS	-	expression tag	UNP A0A0K0YAS1
F	223	GLY	-	expression tag	UNP A0A0K0YAS1
F	224	GLY	-	expression tag	UNP A0A0K0YAS1
F	225	GLY	-	expression tag	UNP A0A0K0YAS1
F	226	SER	-	expression tag	UNP A0A0K0YAS1
F	227	GLY	-	expression tag	UNP A0A0K0YAS1
F	228	GLY	-	expression tag	UNP A0A0K0YAS1
F	229	GLY	-	expression tag	UNP A0A0K0YAS1
F	230	SER	-	expression tag	UNP A0A0K0YAS1
F	231	HIS	-	expression tag	UNP A0A0K0YAS1
F	232	HIS	-	expression tag	UNP A0A0K0YAS1
F	233	HIS	-	expression tag	UNP A0A0K0YAS1
F	234	HIS	-	expression tag	UNP A0A0K0YAS1
F	235	HIS	-	expression tag	UNP A0A0K0YAS1
F	236	HIS	-	expression tag	UNP A0A0K0YAS1

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	P	3	Total	C	N	O	0	0
			39	22	2	15		
5	Q	3	Total	C	N	O	0	0
			39	22	2	15		
5	S	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		

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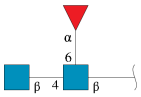
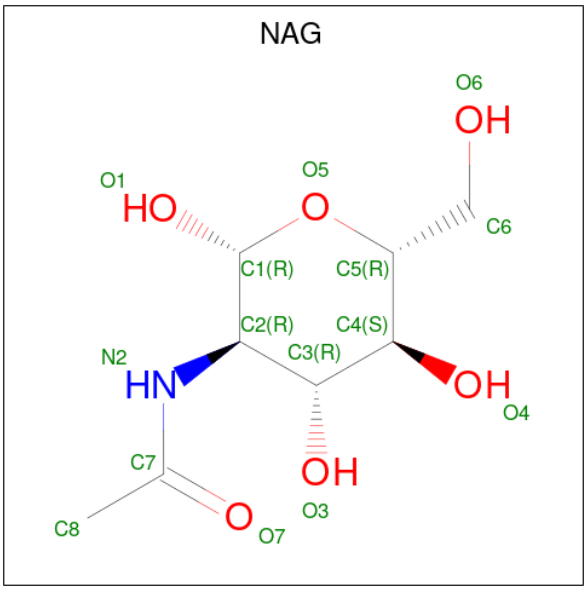
Mol	Chain	Residues	Atoms	AltConf	Trace
5	U	3	Total C N O 39 22 2 15	0	0
5	W	3	Total C N O 39 22 2 15	0	0
5	X	3	Total C N O 39 22 2 15	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
6	N	3	Total C N O 38 22 2 14	0	0
6	R	3	Total C N O 38 22 2 14	0	0
6	V	3	Total C N O 38 22 2 14	0	0

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



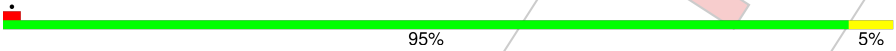
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7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

3 Residue-property plots

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.

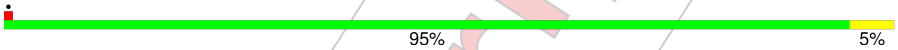
- Molecule 1: NI06063_d30_103 Fab heavy chain

Chain H:



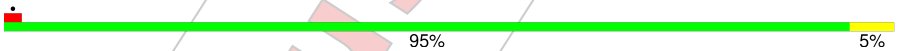
- Molecule 1: NI06063_d30_103 Fab heavy chain

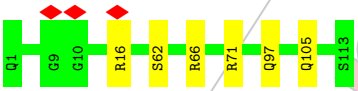
Chain G:



- Molecule 1: NI06063_d30_103 Fab heavy chain

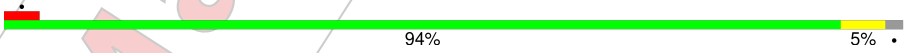
Chain I:

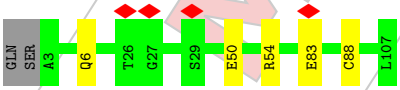




- Molecule 2: NI06063_d30_103 Fab light chain

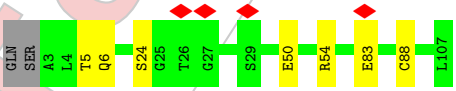
Chain L:





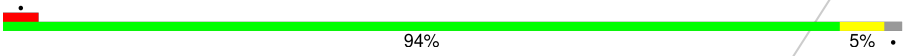
- Molecule 2: NI06063_d30_103 Fab light chain

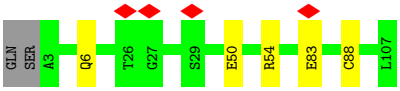
Chain J:



• Molecule 2: NI06063_d30_103 Fab light chain

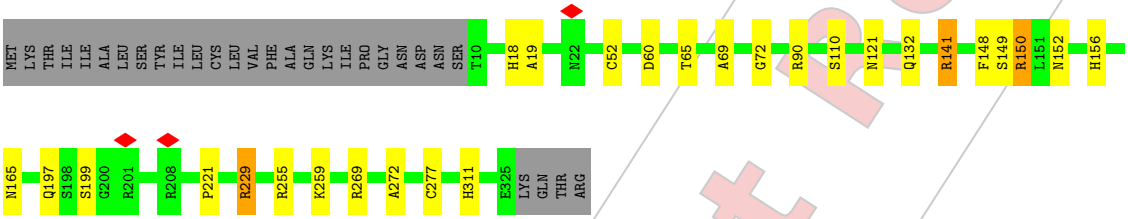
Chain K:





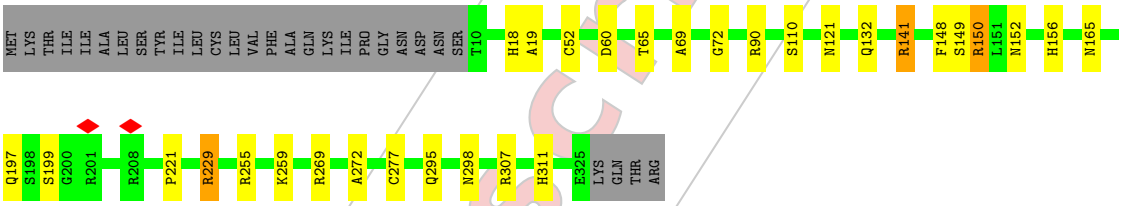
• Molecule 3: Hemagglutinin HA1

Chain A:



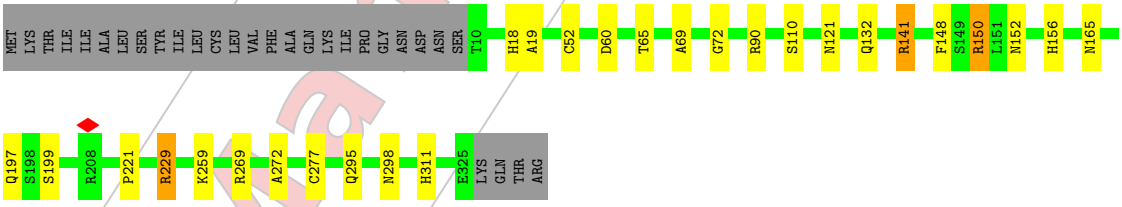
• Molecule 3: Hemagglutinin HA1

Chain C:



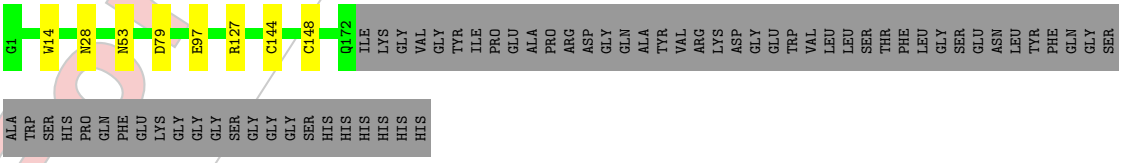
• Molecule 3: Hemagglutinin HA1

Chain D:



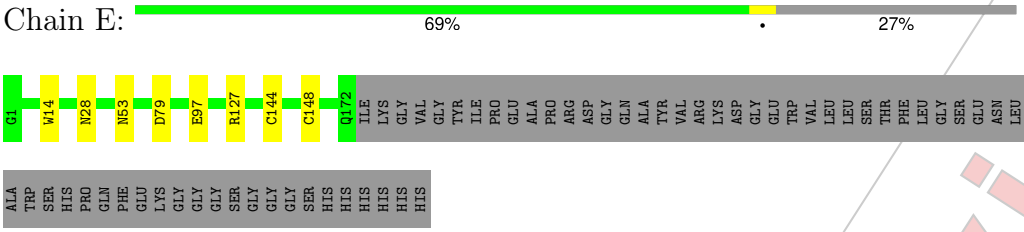
• Molecule 4: Hemagglutinin HA2

Chain B:



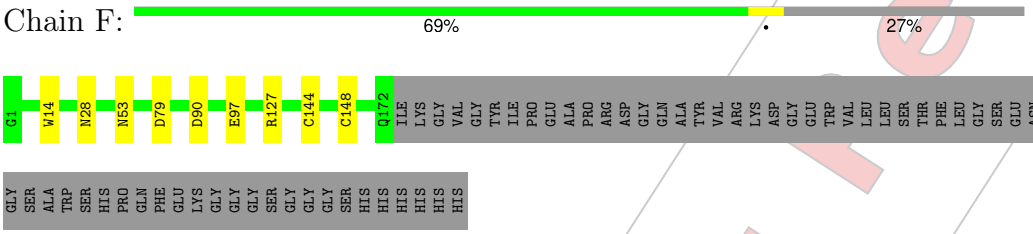
• Molecule 4: Hemagglutinin HA2

Chain E:



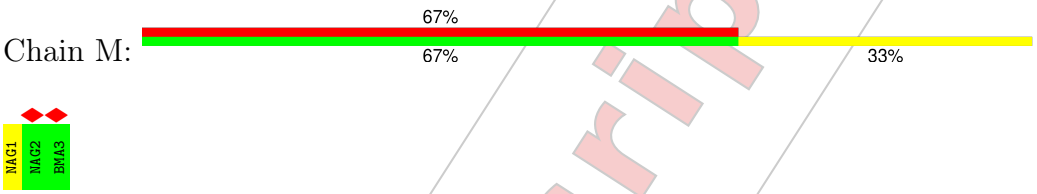
• Molecule 4: Hemagglutinin HA2

Chain F:



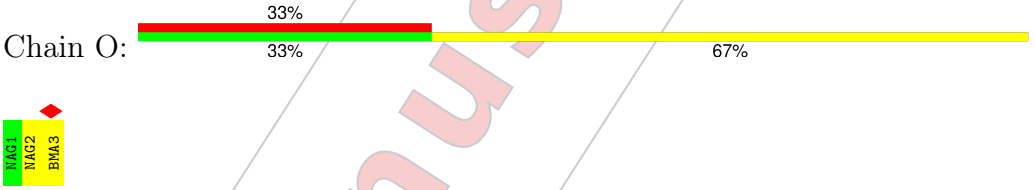
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain O:

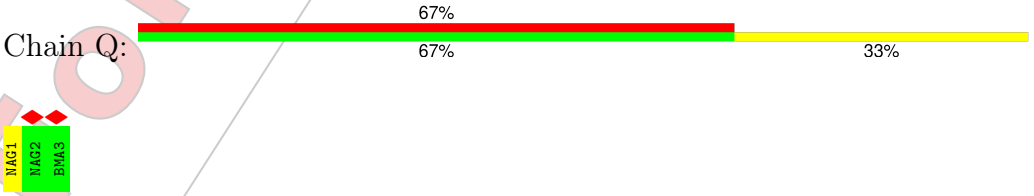


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

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

Chain Q:



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

Chain S:

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

Chain T:

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

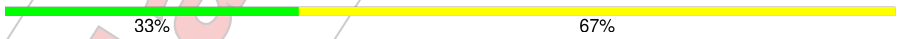
Chain U:

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

Chain W:

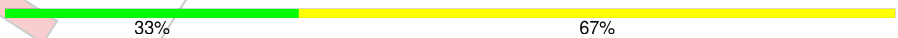
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain N:



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

Chain R:

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

Chain V:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	156709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45.09	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	190000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.427	Depositor
Minimum map value	-0.230	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	315.91998, 315.91998, 315.91998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71799994, 0.71799994, 0.71799994	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, FUC, 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	G	0.30	0/977	0.63	0/1322
1	H	0.30	0/977	0.62	0/1322
1	I	0.30	0/977	0.62	0/1322
2	J	0.29	0/787	0.62	0/1063
2	K	0.29	0/787	0.62	0/1063
2	L	0.29	0/787	0.62	0/1063
3	A	0.30	0/2528	0.65	0/3439
3	C	0.30	0/2528	0.65	0/3439
3	D	0.30	0/2528	0.65	0/3439
4	B	0.27	0/1412	0.58	0/1895
4	E	0.27	0/1412	0.58	0/1895
4	F	0.28	0/1412	0.58	0/1895
All	All	0.29	0/17112	0.63	0/23157

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	J	0	1
2	K	0	1
2	L	0	1
3	A	0	4
3	C	0	4
3	D	0	4
4	B	0	1
4	E	0	1
4	F	0	1
All	All	0	18

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	141	ARG	Sidechain
3	A	150	ARG	Sidechain
3	A	229	ARG	Sidechain
3	A	269	ARG	Sidechain
4	B	127	ARG	Sidechain
3	C	141	ARG	Sidechain
3	C	150	ARG	Sidechain
3	C	229	ARG	Sidechain
3	C	269	ARG	Sidechain
3	D	141	ARG	Sidechain
3	D	150	ARG	Sidechain
3	D	229	ARG	Sidechain
3	D	269	ARG	Sidechain
4	E	127	ARG	Sidechain
4	F	127	ARG	Sidechain
2	J	54	ARG	Sidechain
2	K	54	ARG	Sidechain
2	L	54	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	951	0	893	2	0
1	H	951	0	893	2	0
1	I	951	0	893	2	0
2	J	771	0	747	2	0
2	K	771	0	747	1	0
2	L	771	0	747	1	0
3	A	2471	0	2418	12	0
3	C	2471	0	2418	14	0
3	D	2471	0	2418	12	0
4	B	1388	0	1318	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1388	0	1318	4	0
4	F	1388	0	1318	5	0
5	M	39	0	34	0	0
5	O	39	0	34	0	0
5	P	39	0	34	0	0
5	Q	39	0	34	0	0
5	S	39	0	34	0	0
5	T	39	0	34	0	0
5	U	39	0	34	0	0
5	W	39	0	34	0	0
5	X	39	0	34	0	0
6	N	38	0	34	0	0
6	R	38	0	34	0	0
6	V	38	0	34	0	0
7	A	84	0	78	1	0
7	B	14	0	13	0	0
7	C	84	0	78	1	0
7	D	84	0	78	1	0
7	E	14	0	13	0	0
7	F	14	0	13	0	0
All	All	17502	0	16809	54	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 2.

All (54) 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:I:62:SER:O	1:I:66:ARG:NH2	2.21	0.73
1:H:62:SER:O	1:H:66:ARG:NH2	2.21	0.73
1:G:62:SER:O	1:G:66:ARG:NH2	2.21	0.73
4:B:79:ASP:OD2	3:D:110:SER:OG	2.12	0.64
3:A:221:PRO:O	3:A:229:ARG:NH2	2.31	0.64
3:C:221:PRO:O	3:C:229:ARG:NH2	2.31	0.63
3:D:221:PRO:O	3:D:229:ARG:NH2	2.31	0.62
3:A:110:SER:OG	4:E:79:ASP:OD2	2.13	0.59
3:C:90:ARG:NH1	3:C:272:ALA:O	2.39	0.56
3:A:90:ARG:NH1	3:A:272:ALA:O	2.39	0.54
3:D:90:ARG:NH1	3:D:272:ALA:O	2.39	0.54
2:L:6:GLN:NE2	2:L:88:CYS:SG	2.80	0.54
3:C:110:SER:OG	4:F:79:ASP:OD2	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:6:GLN:NE2	2:K:88:CYS:SG	2.81	0.53
2:J:6:GLN:NE2	2:J:88:CYS:SG	2.81	0.53
4:E:28:ASN:ND2	4:E:144:CYS:O	2.43	0.52
4:F:28:ASN:ND2	4:F:144:CYS:O	2.43	0.51
4:B:28:ASN:ND2	4:B:144:CYS:O	2.43	0.51
3:D:72:GLY:O	3:D:141:ARG:NH2	2.44	0.51
3:C:72:GLY:O	3:C:141:ARG:NH2	2.44	0.50
1:I:97:GLN:NE2	4:F:53:ASN:OD1	2.43	0.49
3:A:72:GLY:O	3:A:141:ARG:NH2	2.44	0.49
3:D:132:GLN:OE1	3:D:152:ASN:ND2	2.46	0.49
1:G:97:GLN:NE2	4:E:53:ASN:OD1	2.43	0.49
1:H:97:GLN:NE2	4:B:53:ASN:OD1	2.43	0.49
3:A:132:GLN:OE1	3:A:152:ASN:ND2	2.46	0.48
3:C:132:GLN:OE1	3:C:152:ASN:ND2	2.47	0.48
3:D:60:ASP:OD2	3:D:90:ARG:NH2	2.47	0.48
3:C:52:CYS:SG	3:C:277:CYS:N	2.88	0.46
3:A:60:ASP:OD2	3:A:90:ARG:NH2	2.46	0.46
3:A:52:CYS:SG	3:A:277:CYS:N	2.88	0.46
3:D:52:CYS:SG	3:D:277:CYS:N	2.88	0.45
3:C:60:ASP:OD2	3:C:90:ARG:NH2	2.46	0.44
3:C:65:THR:O	3:C:69:ALA:N	2.52	0.43
3:A:19:ALA:N	4:B:14:TRP:O	2.51	0.42
3:A:197:GLN:NE2	3:A:199:SER:O	2.52	0.42
3:D:121:ASN:OD1	3:D:259:LYS:NZ	2.53	0.42
3:D:19:ALA:N	4:F:14:TRP:O	2.51	0.42
3:C:197:GLN:NE2	3:C:199:SER:O	2.52	0.42
3:C:19:ALA:N	4:E:14:TRP:O	2.50	0.41
3:A:149:SER:O	3:A:255:ARG:NE	2.51	0.41
3:C:121:ASN:OD1	3:C:259:LYS:NZ	2.53	0.41
3:D:65:THR:O	3:D:69:ALA:N	2.52	0.41
3:C:295:GLN:NE2	3:C:298:ASN:O	2.53	0.41
3:D:295:GLN:NE2	3:D:298:ASN:O	2.54	0.41
2:J:5:THR:N	2:J:24:SER:O	2.54	0.41
3:A:121:ASN:OD1	3:A:259:LYS:NZ	2.53	0.41
3:A:65:THR:O	3:A:69:ALA:N	2.52	0.41
7:A:403:NAG:H83	7:A:403:NAG:H3	2.03	0.41
3:C:149:SER:O	3:C:255:ARG:NE	2.52	0.41
3:C:307:ARG:NH2	4:F:90:ASP:OD2	2.52	0.40
3:D:197:GLN:NE2	3:D:199:SER:O	2.52	0.40
7:D:403:NAG:H3	7:D:403:NAG:H83	2.04	0.40
7:C:403:NAG:H83	7:C:403:NAG:H3	2.03	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	G	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
1	H	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
1	I	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
2	J	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
2	K	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
2	L	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
3	A	314/345 (91%)	308 (98%)	6 (2%)	0	100	100
3	C	314/345 (91%)	308 (98%)	6 (2%)	0	100	100
3	D	314/345 (91%)	309 (98%)	5 (2%)	0	100	100
4	B	170/236 (72%)	168 (99%)	2 (1%)	0	100	100
4	E	170/236 (72%)	168 (99%)	2 (1%)	0	100	100
4	F	170/236 (72%)	168 (99%)	2 (1%)	0	100	100
All	All	2124/2433 (87%)	2053 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	97/98 (99%)	94 (97%)	3 (3%)	35	60
1	H	97/98 (99%)	94 (97%)	3 (3%)	35	60
1	I	97/98 (99%)	94 (97%)	3 (3%)	35	60
2	J	85/87 (98%)	83 (98%)	2 (2%)	44	68
2	K	85/87 (98%)	83 (98%)	2 (2%)	44	68
2	L	85/87 (98%)	83 (98%)	2 (2%)	44	68
3	A	280/306 (92%)	274 (98%)	6 (2%)	48	72
3	C	280/306 (92%)	274 (98%)	6 (2%)	48	72
3	D	280/306 (92%)	274 (98%)	6 (2%)	48	72
4	B	145/194 (75%)	143 (99%)	2 (1%)	62	81
4	E	145/194 (75%)	143 (99%)	2 (1%)	62	81
4	F	145/194 (75%)	143 (99%)	2 (1%)	62	81
All	All	1821/2055 (89%)	1782 (98%)	39 (2%)	49	72

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	16	ARG
1	H	71	ARG
1	H	105	GLN
2	L	50	GLU
2	L	83	GLU
3	A	18	HIS
3	A	148	PHE
3	A	150	ARG
3	A	156	HIS
3	A	165	ASN
3	A	311	HIS
4	B	97	GLU
4	B	148	CYS
1	G	16	ARG
1	G	71	ARG
1	G	105	GLN
2	J	50	GLU
2	J	83	GLU
3	C	18	HIS
3	C	148	PHE
3	C	150	ARG
3	C	156	HIS

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Mol	Chain	Res	Type
3	C	165	ASN
3	C	311	HIS
4	E	97	GLU
4	E	148	CYS
1	I	16	ARG
1	I	71	ARG
1	I	105	GLN
2	K	50	GLU
2	K	83	GLU
3	D	18	HIS
3	D	148	PHE
3	D	150	ARG
3	D	156	HIS
3	D	165	ASN
3	D	311	HIS
4	F	97	GLU
4	F	148	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	M	1	3,5	14,14,15	0.30	0	17,19,21	0.97	2 (11%)
5	NAG	M	2	5	14,14,15	0.34	0	17,19,21	0.53	0
5	BMA	M	3	5	11,11,12	0.53	0	15,15,17	0.75	0
6	NAG	N	1	3,6	14,14,15	0.24	0	17,19,21	0.76	1 (5%)
6	NAG	N	2	6	14,14,15	0.37	0	17,19,21	0.85	1 (5%)
6	FUC	N	3	6	10,10,11	0.62	0	14,14,16	0.61	0
5	NAG	O	1	3,5	14,14,15	0.32	0	17,19,21	0.59	0
5	NAG	O	2	5	14,14,15	0.34	0	17,19,21	0.92	2 (11%)
5	BMA	O	3	5	11,11,12	0.61	0	15,15,17	0.80	1 (6%)
5	NAG	P	1	3,5	14,14,15	0.66	0	17,19,21	0.70	0
5	NAG	P	2	5	14,14,15	0.25	0	17,19,21	1.00	2 (11%)
5	BMA	P	3	5	11,11,12	1.83	3 (27%)	15,15,17	1.56	2 (13%)
5	NAG	Q	1	3,5	14,14,15	0.30	0	17,19,21	0.96	2 (11%)
5	NAG	Q	2	5	14,14,15	0.31	0	17,19,21	0.52	0
5	BMA	Q	3	5	11,11,12	0.52	0	15,15,17	0.74	0
6	NAG	R	1	3,6	14,14,15	0.22	0	17,19,21	0.77	1 (5%)
6	NAG	R	2	6	14,14,15	0.42	0	17,19,21	0.83	1 (5%)
6	FUC	R	3	6	10,10,11	0.62	0	14,14,16	0.61	0
5	NAG	S	1	3,5	14,14,15	0.32	0	17,19,21	0.59	0
5	NAG	S	2	5	14,14,15	0.33	0	17,19,21	0.91	2 (11%)
5	BMA	S	3	5	11,11,12	0.61	0	15,15,17	0.81	1 (6%)
5	NAG	T	1	3,5	14,14,15	0.65	0	17,19,21	0.70	0
5	NAG	T	2	5	14,14,15	0.25	0	17,19,21	1.00	2 (11%)
5	BMA	T	3	5	11,11,12	1.86	3 (27%)	15,15,17	1.55	2 (13%)
5	NAG	U	1	3,5	14,14,15	0.32	0	17,19,21	0.97	2 (11%)
5	NAG	U	2	5	14,14,15	0.30	0	17,19,21	0.53	0
5	BMA	U	3	5	11,11,12	0.53	0	15,15,17	0.74	0
6	NAG	V	1	3,6	14,14,15	0.23	0	17,19,21	0.76	1 (5%)
6	NAG	V	2	6	14,14,15	0.38	0	17,19,21	0.85	1 (5%)
6	FUC	V	3	6	10,10,11	0.63	0	14,14,16	0.61	0
5	NAG	W	1	3,5	14,14,15	0.33	0	17,19,21	0.59	0
5	NAG	W	2	5	14,14,15	0.33	0	17,19,21	0.92	2 (11%)
5	BMA	W	3	5	11,11,12	0.62	0	15,15,17	0.81	1 (6%)
5	NAG	X	1	3,5	14,14,15	0.65	0	17,19,21	0.70	0
5	NAG	X	2	5	14,14,15	0.25	0	17,19,21	1.00	2 (11%)
5	BMA	X	3	5	11,11,12	1.84	3 (27%)	15,15,17	1.57	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	X	3	5	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	3	BMA	O5-C1	4.51	1.51	1.43
5	P	3	BMA	O5-C1	4.46	1.51	1.43
5	X	3	BMA	O5-C1	4.45	1.51	1.43
5	X	3	BMA	O5-C5	2.46	1.48	1.43
5	T	3	BMA	O5-C5	2.44	1.48	1.43
5	P	3	BMA	O5-C5	2.43	1.48	1.43
5	T	3	BMA	C1-C2	2.35	1.57	1.52
5	X	3	BMA	C1-C2	2.31	1.57	1.52
5	P	3	BMA	C1-C2	2.28	1.57	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	3	BMA	C1-O5-C5	4.23	117.85	112.19
5	T	3	BMA	C1-O5-C5	4.21	117.83	112.19
5	P	3	BMA	C1-O5-C5	4.18	117.78	112.19
5	M	1	NAG	C2-N2-C7	2.92	126.81	122.90
5	U	1	NAG	C2-N2-C7	2.92	126.81	122.90
5	Q	1	NAG	C2-N2-C7	2.87	126.75	122.90
5	X	2	NAG	C2-N2-C7	2.86	126.73	122.90
5	T	2	NAG	C2-N2-C7	2.84	126.71	122.90
5	P	2	NAG	C2-N2-C7	2.83	126.69	122.90
5	O	2	NAG	C2-N2-C7	2.81	126.67	122.90
5	W	2	NAG	C2-N2-C7	2.79	126.64	122.90
5	S	2	NAG	C2-N2-C7	2.78	126.62	122.90
6	V	2	NAG	C2-N2-C7	2.77	126.61	122.90
6	N	2	NAG	C2-N2-C7	2.75	126.59	122.90
6	R	1	NAG	C1-O5-C5	2.69	115.80	112.19
6	R	2	NAG	C2-N2-C7	2.68	126.49	122.90
6	V	1	NAG	C1-O5-C5	2.64	115.73	112.19
6	N	1	NAG	C1-O5-C5	2.63	115.71	112.19
5	X	3	BMA	C3-C4-C5	2.40	114.59	110.23
5	P	3	BMA	C3-C4-C5	2.38	114.55	110.23
5	P	2	NAG	C1-O5-C5	2.34	115.33	112.19
5	T	3	BMA	C3-C4-C5	2.33	114.46	110.23
5	T	2	NAG	C1-O5-C5	2.33	115.31	112.19
5	X	2	NAG	C1-O5-C5	2.32	115.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	3	BMA	C1-O5-C5	2.22	115.16	112.19
5	W	3	BMA	C1-O5-C5	2.20	115.13	112.19
5	O	3	BMA	C1-O5-C5	2.20	115.13	112.19
5	M	1	NAG	C1-O5-C5	2.06	114.95	112.19
5	O	2	NAG	C1-O5-C5	2.05	114.93	112.19
5	W	2	NAG	C1-O5-C5	2.03	114.91	112.19
5	Q	1	NAG	C1-O5-C5	2.03	114.91	112.19
5	U	1	NAG	C1-O5-C5	2.03	114.90	112.19
5	S	2	NAG	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	P	2	NAG	C8-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
5	X	2	NAG	C8-C7-N2-C2
5	X	2	NAG	O7-C7-N2-C2

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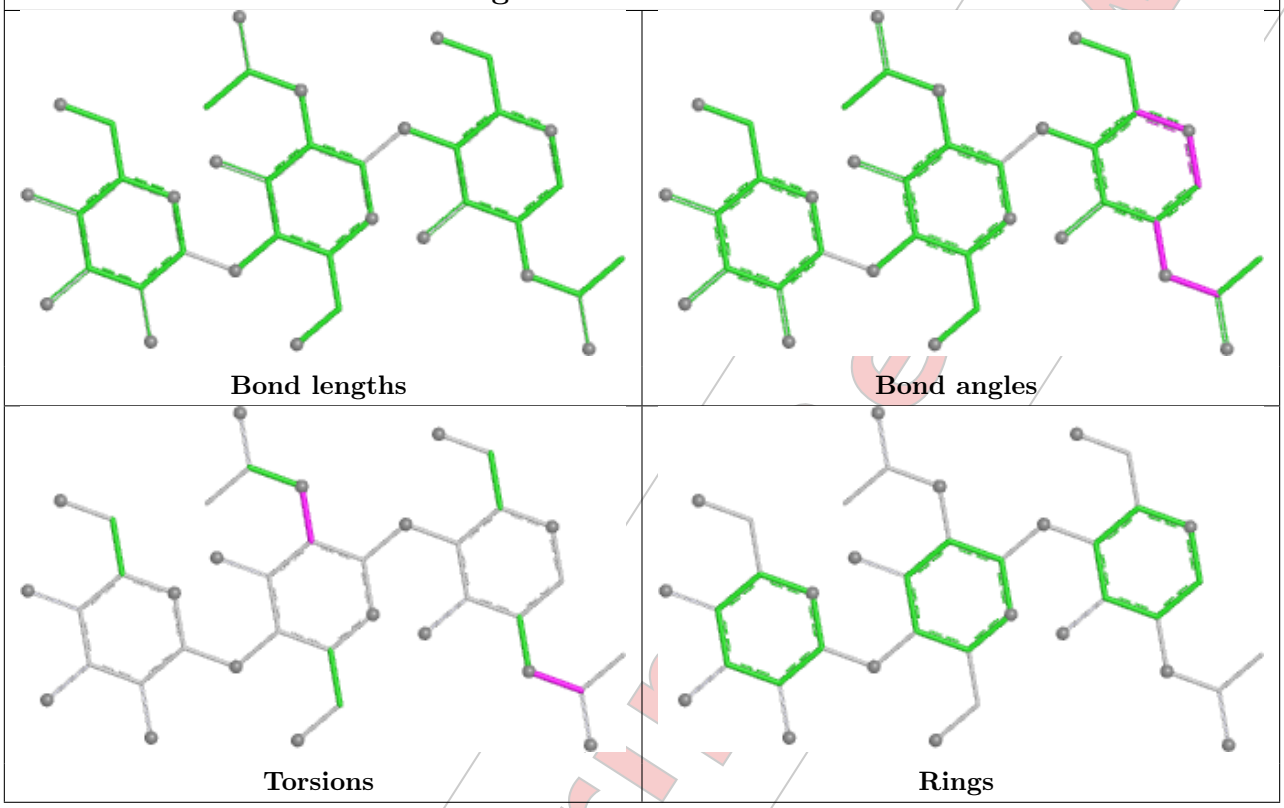
Mol	Chain	Res	Type	Atoms
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	R	2	NAG	C8-C7-N2-C2
6	R	2	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
5	P	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	X	3	BMA	C4-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	M	2	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
5	U	2	NAG	C1-C2-N2-C7
6	N	1	NAG	C1-C2-N2-C7
6	R	1	NAG	C1-C2-N2-C7
6	V	1	NAG	C1-C2-N2-C7
6	R	1	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	U	2	NAG	C3-C2-N2-C7
6	N	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7
6	V	1	NAG	C3-C2-N2-C7
6	R	1	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6

There are no ring outliers.

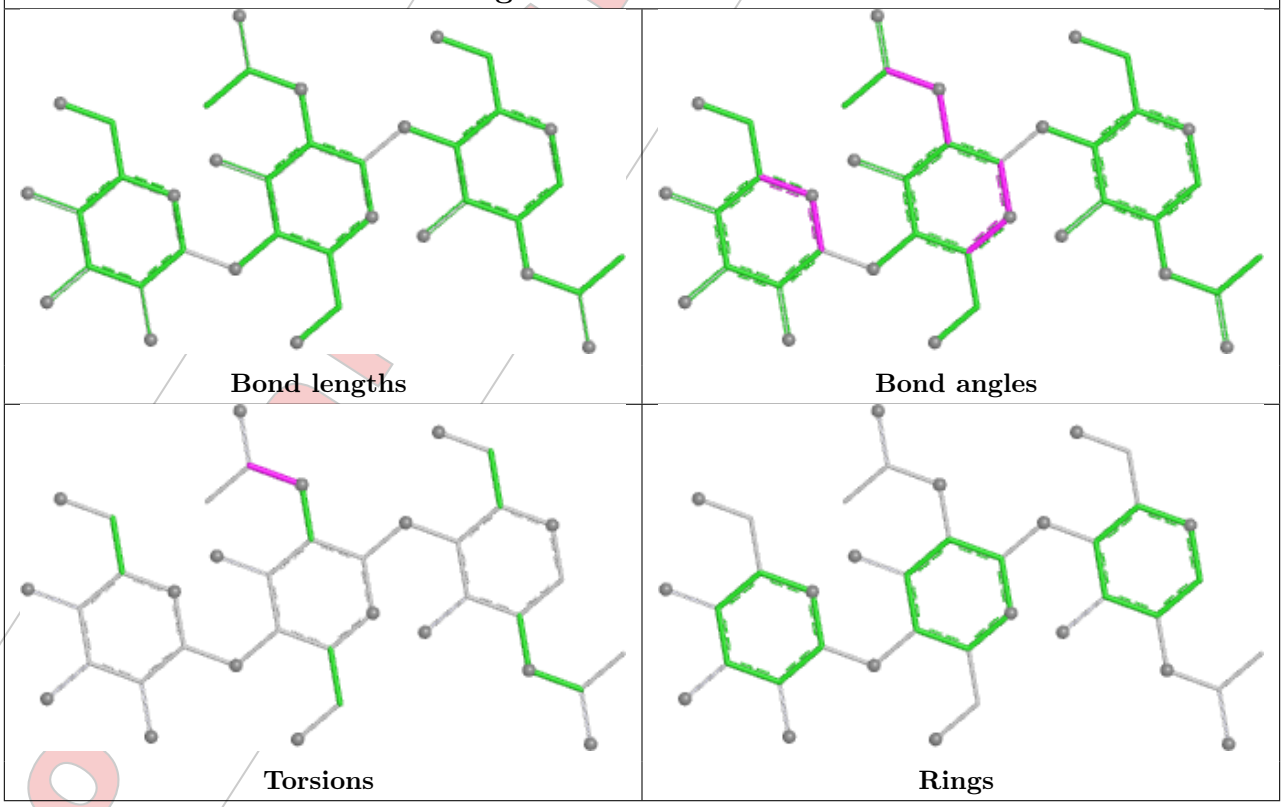
No monomer is involved in short contacts.

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

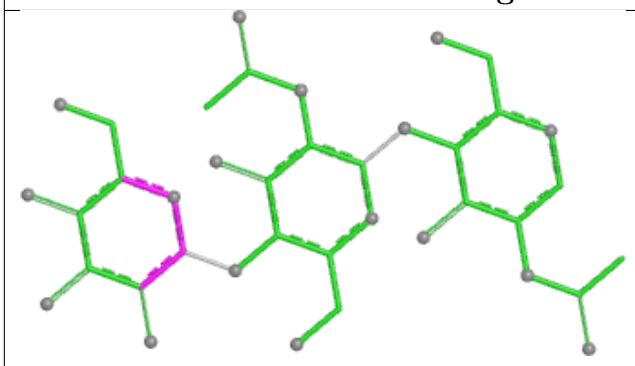
Oligosaccharide Chain M



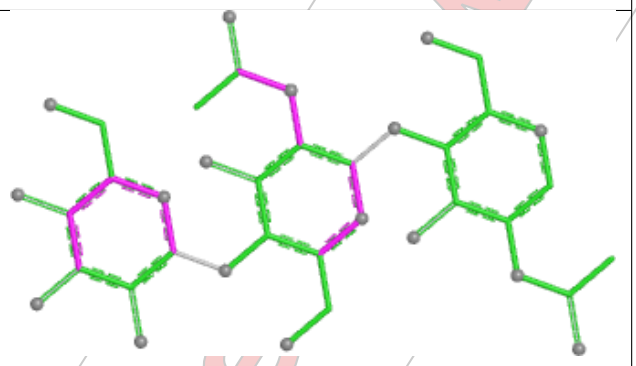
Oligosaccharide Chain O



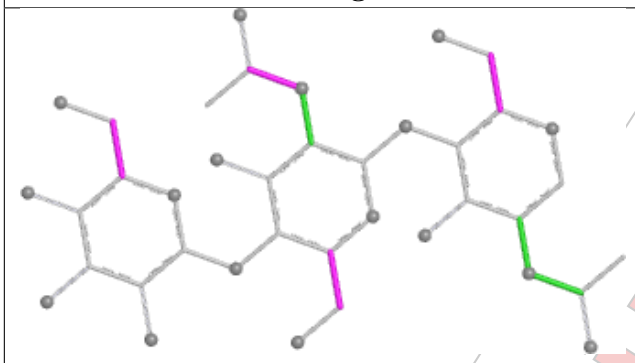
Oligosaccharide Chain P



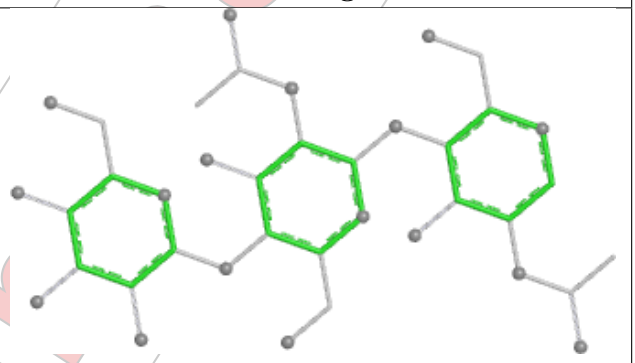
Bond lengths



Bond angles

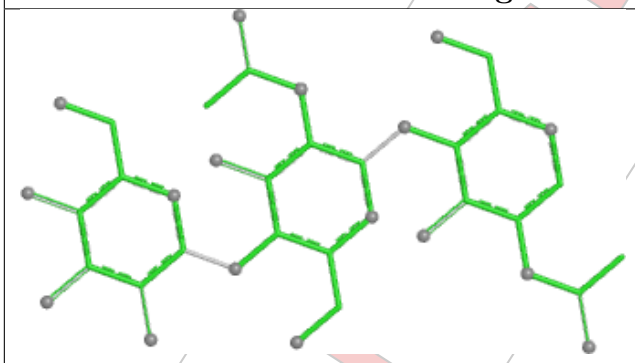


Torsions

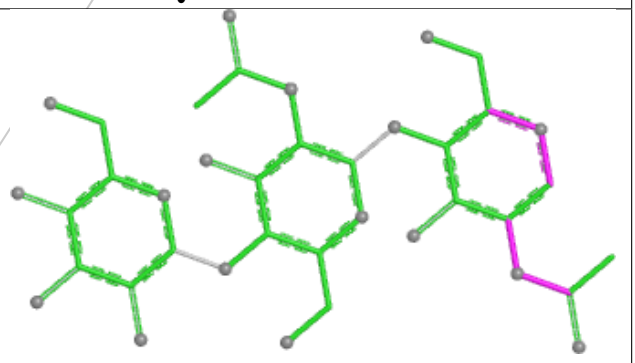


Rings

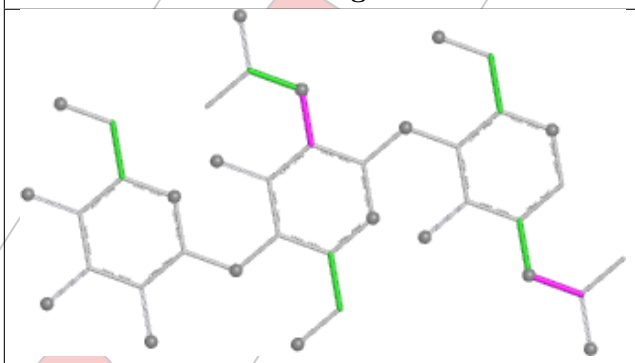
Oligosaccharide Chain Q



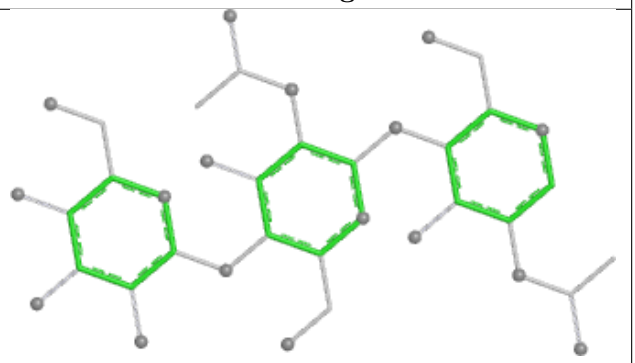
Bond lengths



Bond angles

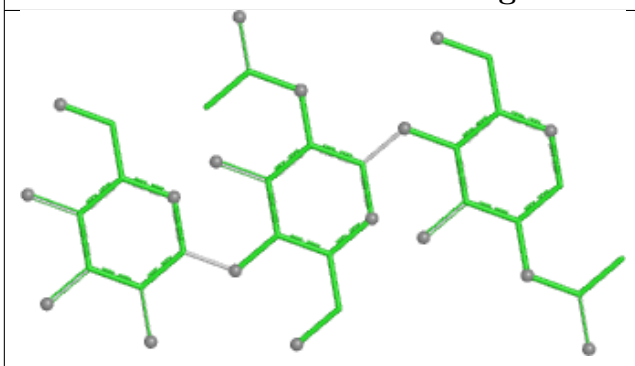


Torsions

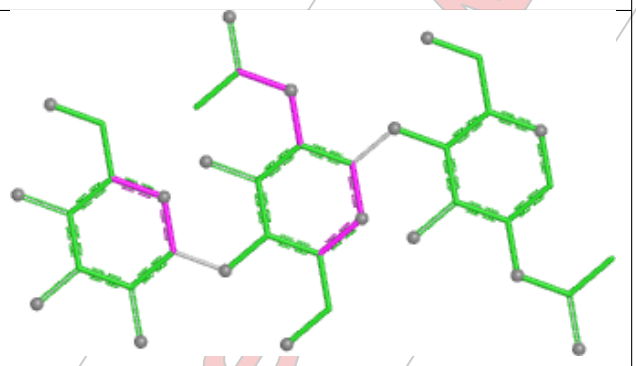


Rings

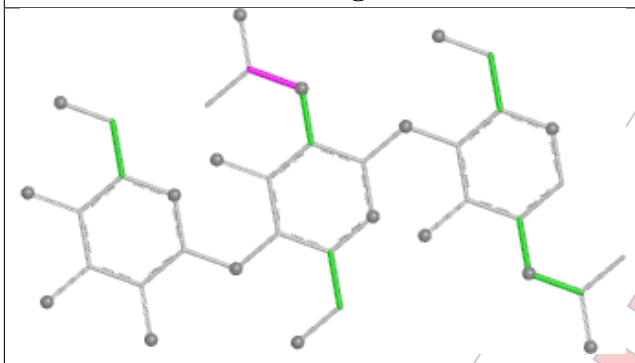
Oligosaccharide Chain S



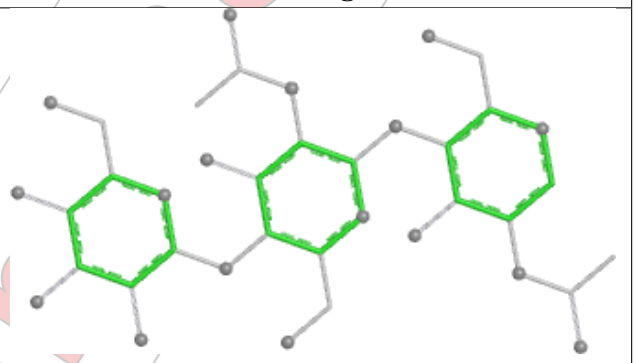
Bond lengths



Bond angles

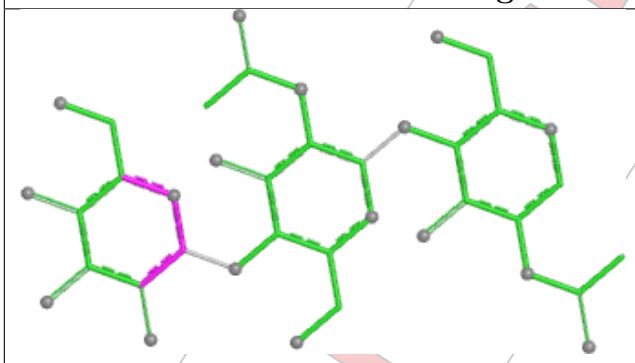


Torsions

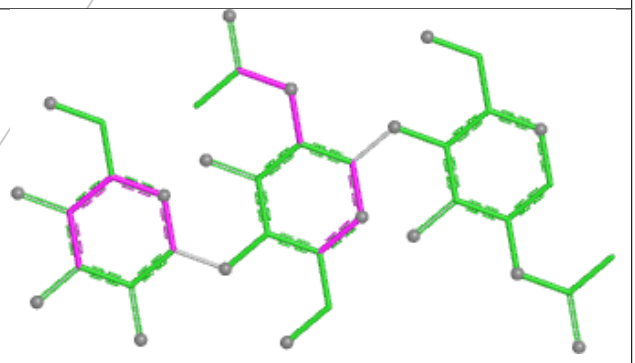


Rings

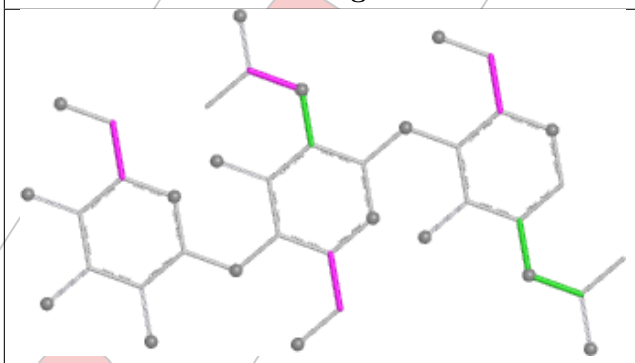
Oligosaccharide Chain T



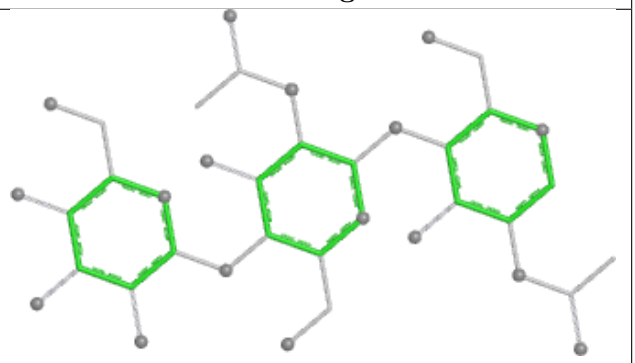
Bond lengths



Bond angles

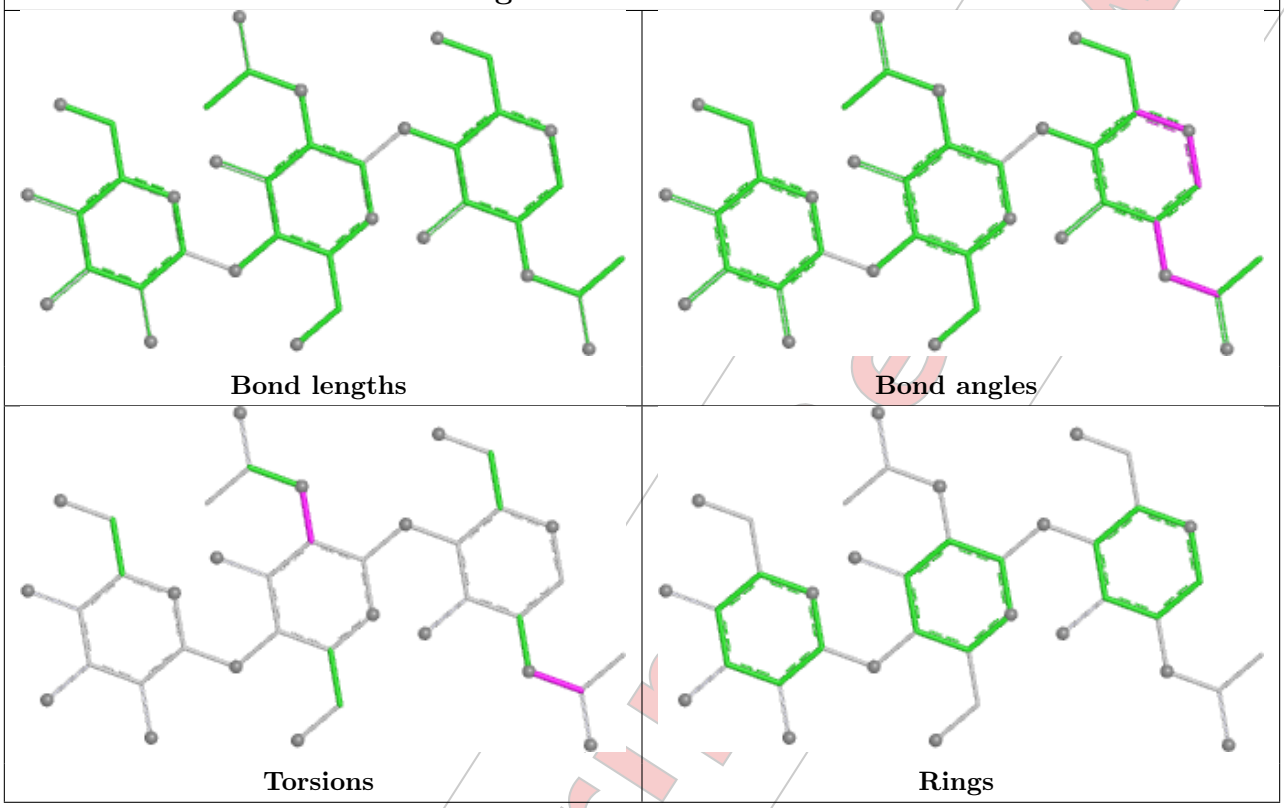


Torsions

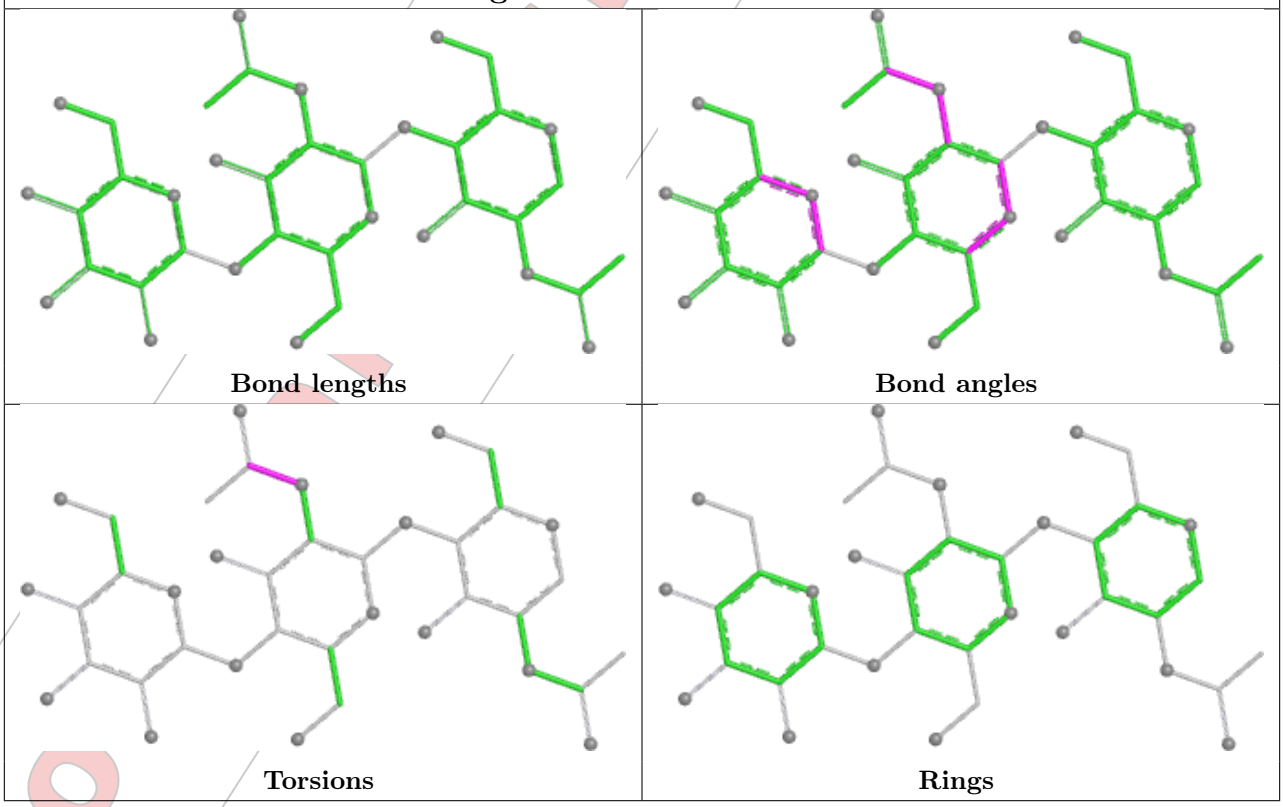


Rings

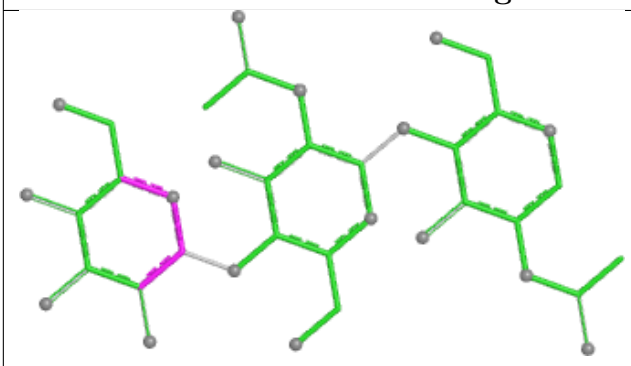
Oligosaccharide Chain U



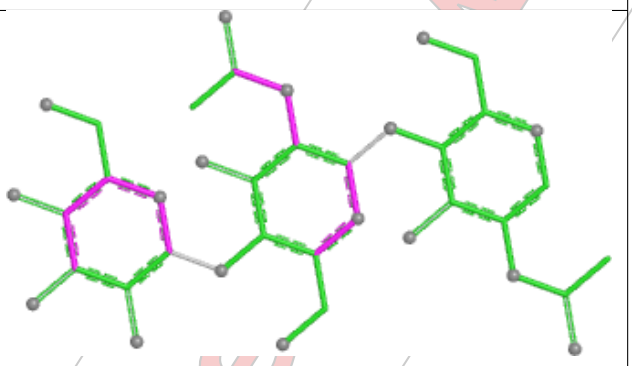
Oligosaccharide Chain W



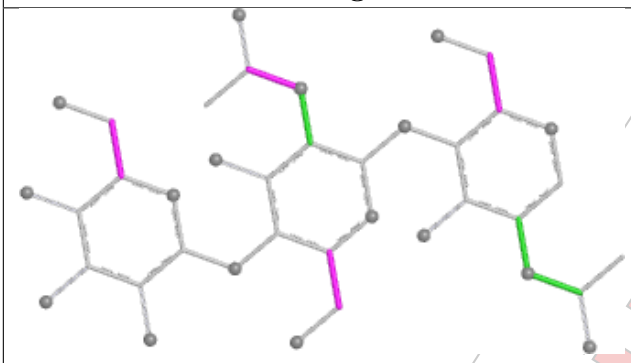
Oligosaccharide Chain X



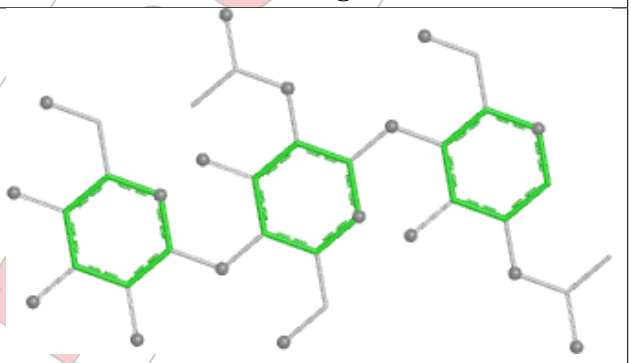
Bond lengths



Bond angles

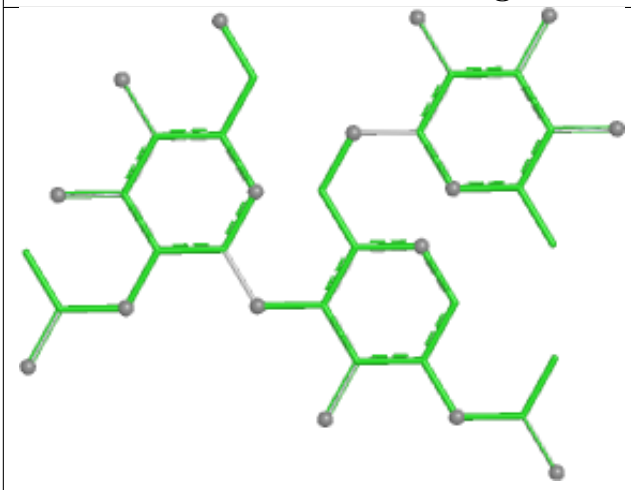


Torsions

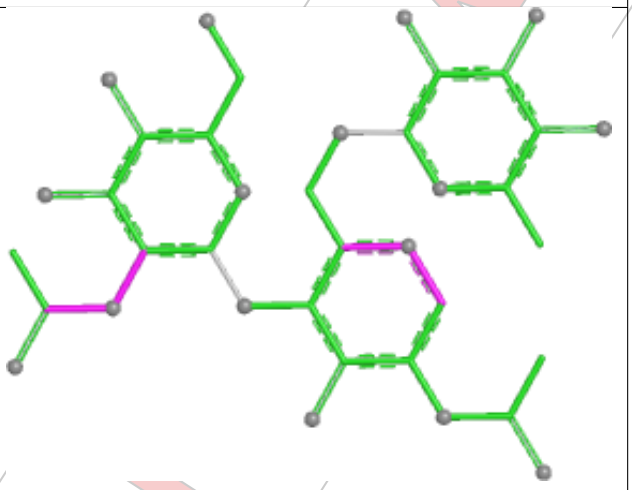


Rings

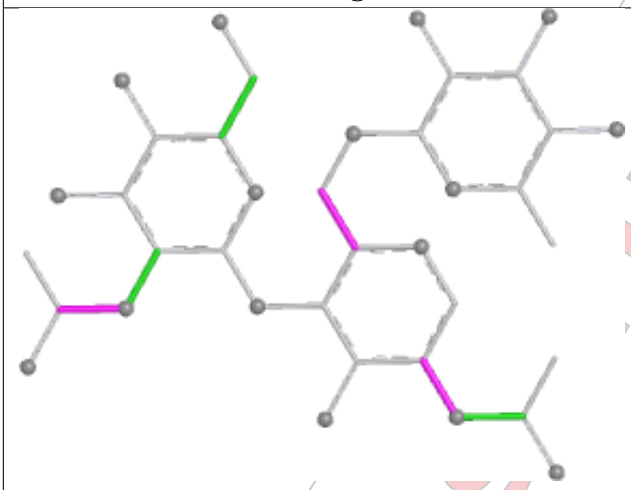
Oligosaccharide Chain N



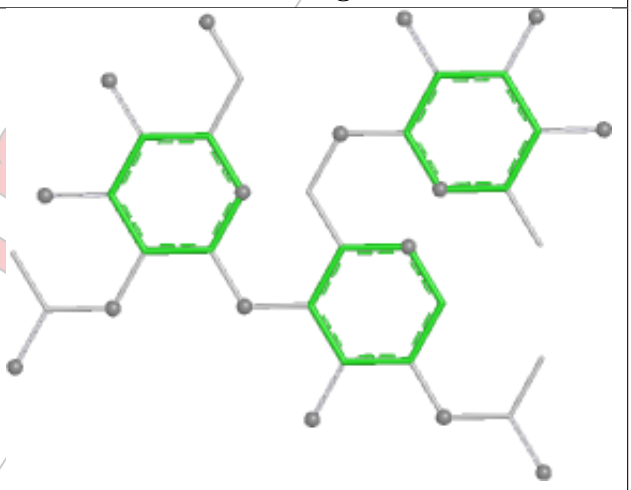
Bond lengths



Bond angles

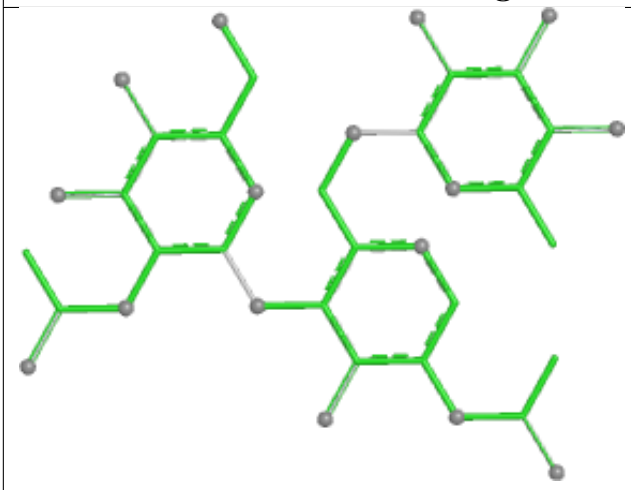


Torsions

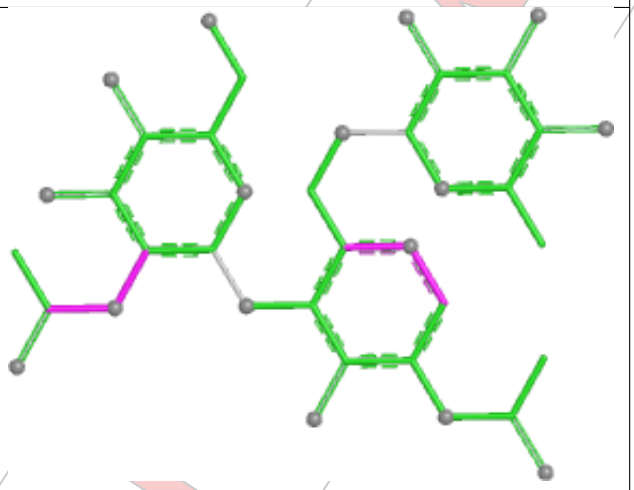


Rings

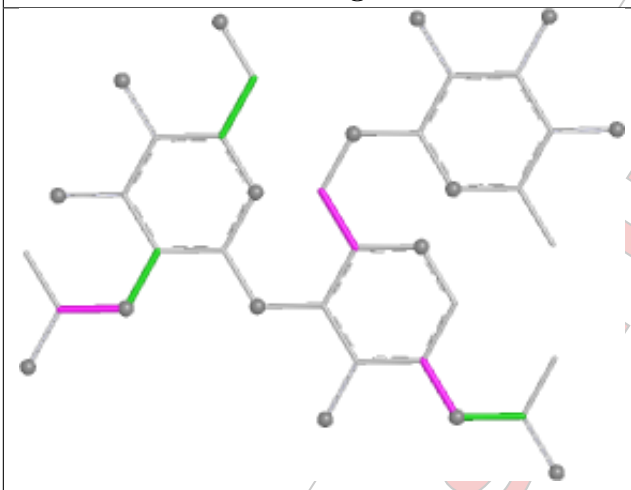
Oligosaccharide Chain R



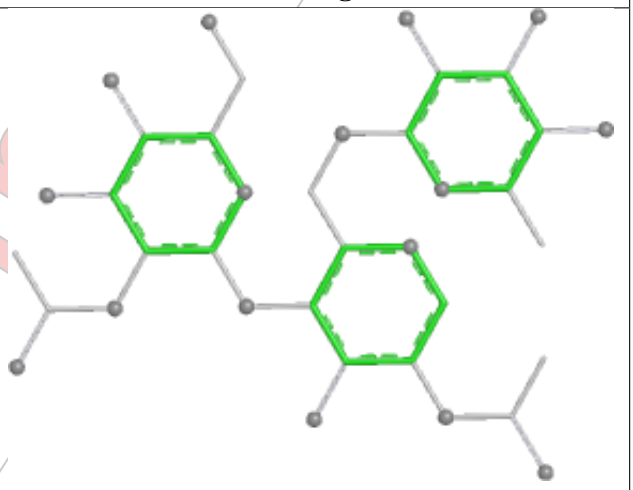
Bond lengths



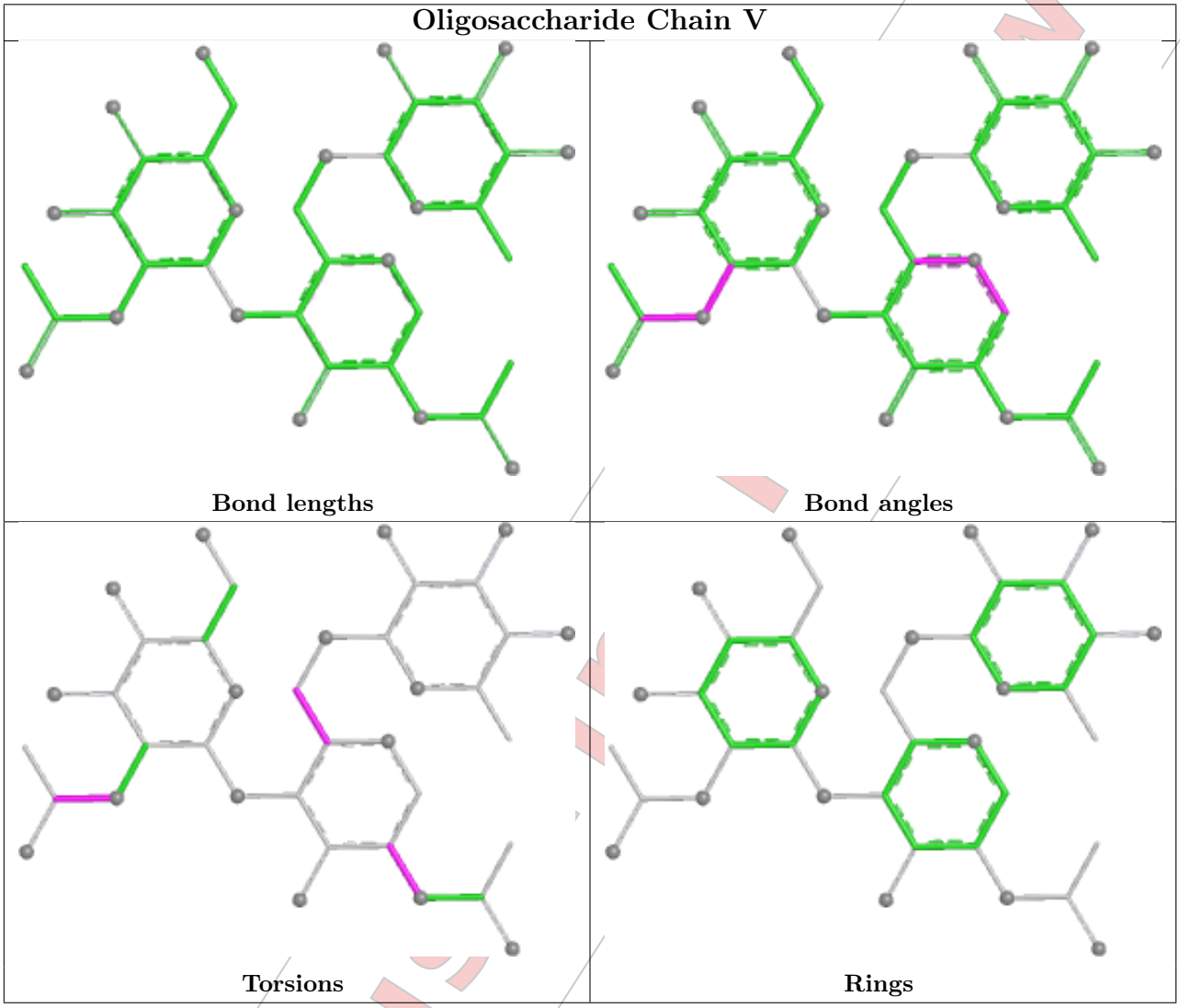
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

21 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	C	401	3	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	D	401	3	14,14,15	0.32	0	17,19,21	0.48	0
7	NAG	A	401	3	14,14,15	0.31	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	B	301	4	14,14,15	0.35	0	17,19,21	0.88	1 (5%)
7	NAG	C	402	3	14,14,15	0.35	0	17,19,21	0.67	1 (5%)
7	NAG	D	402	3	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
7	NAG	C	404	3	14,14,15	0.25	0	17,19,21	0.51	0
7	NAG	C	406	3	14,14,15	0.34	0	17,19,21	0.88	1 (5%)
7	NAG	A	404	3	14,14,15	0.25	0	17,19,21	0.51	0
7	NAG	E	301	4	14,14,15	0.35	0	17,19,21	0.88	1 (5%)
7	NAG	A	403	3	14,14,15	0.34	0	17,19,21	1.49	2 (11%)
7	NAG	F	301	4	14,14,15	0.35	0	17,19,21	0.88	1 (5%)
7	NAG	C	405	3	14,14,15	0.31	0	17,19,21	0.52	0
7	NAG	A	406	3	14,14,15	0.35	0	17,19,21	0.88	1 (5%)
7	NAG	D	403	3	14,14,15	0.34	0	17,19,21	1.49	2 (11%)
7	NAG	A	402	3	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
7	NAG	C	403	3	14,14,15	0.34	0	17,19,21	1.49	2 (11%)
7	NAG	D	406	3	14,14,15	0.35	0	17,19,21	0.88	1 (5%)
7	NAG	D	405	3	14,14,15	0.32	0	17,19,21	0.52	0
7	NAG	D	404	3	14,14,15	0.26	0	17,19,21	0.51	0
7	NAG	A	405	3	14,14,15	0.31	0	17,19,21	0.52	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	C	401	3	-	2/6/23/26	0/1/1/1
7	NAG	D	401	3	-	2/6/23/26	0/1/1/1
7	NAG	A	401	3	-	2/6/23/26	0/1/1/1
7	NAG	B	301	4	-	4/6/23/26	0/1/1/1
7	NAG	C	402	3	-	2/6/23/26	0/1/1/1
7	NAG	D	402	3	-	2/6/23/26	0/1/1/1
7	NAG	C	404	3	-	0/6/23/26	0/1/1/1
7	NAG	C	406	3	-	3/6/23/26	0/1/1/1
7	NAG	A	404	3	-	0/6/23/26	0/1/1/1
7	NAG	E	301	4	-	4/6/23/26	0/1/1/1
7	NAG	A	403	3	-	6/6/23/26	0/1/1/1
7	NAG	F	301	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	405	3	-	3/6/23/26	0/1/1/1
7	NAG	A	406	3	-	3/6/23/26	0/1/1/1
7	NAG	D	403	3	-	6/6/23/26	0/1/1/1
7	NAG	A	402	3	-	2/6/23/26	0/1/1/1
7	NAG	C	403	3	-	6/6/23/26	0/1/1/1
7	NAG	D	406	3	-	3/6/23/26	0/1/1/1
7	NAG	D	405	3	-	3/6/23/26	0/1/1/1
7	NAG	D	404	3	-	0/6/23/26	0/1/1/1
7	NAG	A	405	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	403	NAG	C2-N2-C7	4.80	129.33	122.90
7	C	403	NAG	C2-N2-C7	4.78	129.31	122.90
7	D	403	NAG	C2-N2-C7	4.77	129.30	122.90
7	E	301	NAG	C2-N2-C7	2.99	126.91	122.90
7	B	301	NAG	C2-N2-C7	2.97	126.88	122.90
7	F	301	NAG	C2-N2-C7	2.97	126.88	122.90
7	C	406	NAG	C2-N2-C7	2.94	126.84	122.90
7	D	406	NAG	C2-N2-C7	2.94	126.84	122.90
7	A	406	NAG	C2-N2-C7	2.94	126.84	122.90
7	A	403	NAG	C1-C2-N2	2.64	114.60	110.43
7	D	403	NAG	C1-C2-N2	2.64	114.59	110.43
7	C	403	NAG	C1-C2-N2	2.61	114.55	110.43
7	C	402	NAG	C1-O5-C5	2.42	115.42	112.19
7	A	402	NAG	C1-O5-C5	2.41	115.42	112.19
7	D	402	NAG	C1-O5-C5	2.39	115.39	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	405	NAG	C4-C5-C6-O6
7	C	405	NAG	C4-C5-C6-O6
7	D	405	NAG	C4-C5-C6-O6
7	A	405	NAG	O5-C5-C6-O6
7	C	405	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	D	405	NAG	O5-C5-C6-O6
7	A	403	NAG	O5-C5-C6-O6
7	D	403	NAG	O5-C5-C6-O6
7	C	403	NAG	O5-C5-C6-O6
7	A	403	NAG	C4-C5-C6-O6
7	C	403	NAG	C4-C5-C6-O6
7	D	403	NAG	C4-C5-C6-O6
7	D	401	NAG	O5-C5-C6-O6
7	F	301	NAG	O5-C5-C6-O6
7	A	401	NAG	O5-C5-C6-O6
7	B	301	NAG	O5-C5-C6-O6
7	C	401	NAG	O5-C5-C6-O6
7	E	301	NAG	O5-C5-C6-O6
7	A	403	NAG	C8-C7-N2-C2
7	A	403	NAG	O7-C7-N2-C2
7	A	406	NAG	C8-C7-N2-C2
7	A	406	NAG	O7-C7-N2-C2
7	B	301	NAG	C8-C7-N2-C2
7	B	301	NAG	O7-C7-N2-C2
7	C	403	NAG	C8-C7-N2-C2
7	C	403	NAG	O7-C7-N2-C2
7	C	406	NAG	C8-C7-N2-C2
7	C	406	NAG	O7-C7-N2-C2
7	E	301	NAG	C8-C7-N2-C2
7	E	301	NAG	O7-C7-N2-C2
7	D	403	NAG	C8-C7-N2-C2
7	D	403	NAG	O7-C7-N2-C2
7	D	406	NAG	C8-C7-N2-C2
7	D	406	NAG	O7-C7-N2-C2
7	F	301	NAG	C8-C7-N2-C2
7	F	301	NAG	O7-C7-N2-C2
7	F	301	NAG	C4-C5-C6-O6
7	E	301	NAG	C4-C5-C6-O6
7	B	301	NAG	C4-C5-C6-O6
7	A	401	NAG	C4-C5-C6-O6
7	D	401	NAG	C4-C5-C6-O6
7	C	401	NAG	C4-C5-C6-O6
7	A	406	NAG	O5-C5-C6-O6
7	D	406	NAG	O5-C5-C6-O6
7	C	406	NAG	O5-C5-C6-O6
7	A	402	NAG	C4-C5-C6-O6
7	C	402	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	403	NAG	C1-C2-N2-C7
7	C	403	NAG	C1-C2-N2-C7
7	D	403	NAG	C1-C2-N2-C7
7	D	402	NAG	C4-C5-C6-O6
7	A	405	NAG	C1-C2-N2-C7
7	C	405	NAG	C1-C2-N2-C7
7	D	405	NAG	C1-C2-N2-C7
7	A	403	NAG	C3-C2-N2-C7
7	C	403	NAG	C3-C2-N2-C7
7	D	403	NAG	C3-C2-N2-C7
7	A	402	NAG	O5-C5-C6-O6
7	C	402	NAG	O5-C5-C6-O6
7	D	402	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	403	NAG	1	0
7	D	403	NAG	1	0
7	C	403	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

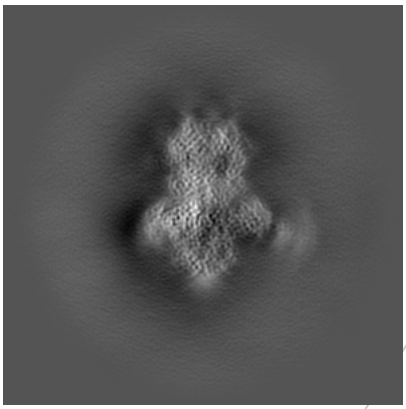
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70233. These allow visual inspection of the internal detail of the map and identification of artifacts.

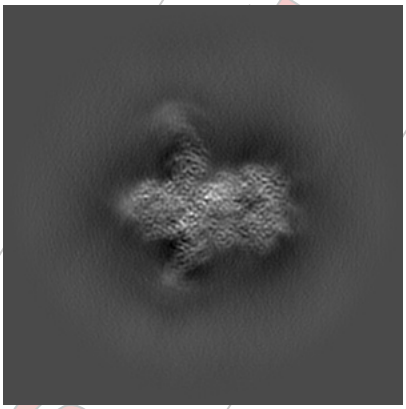
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

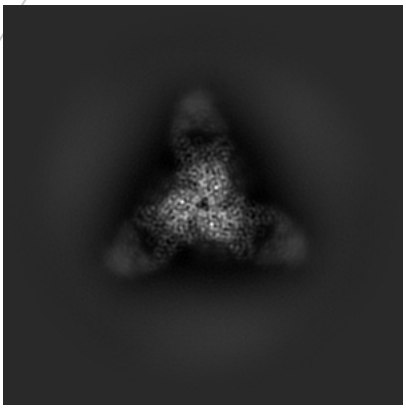
6.1.1 Primary map



X

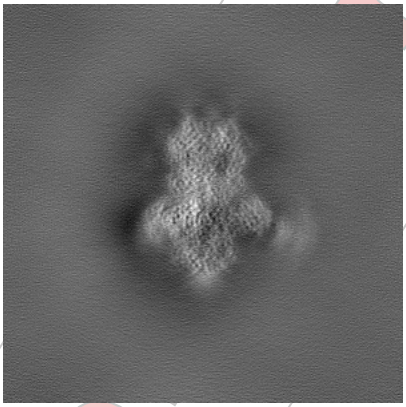


Y

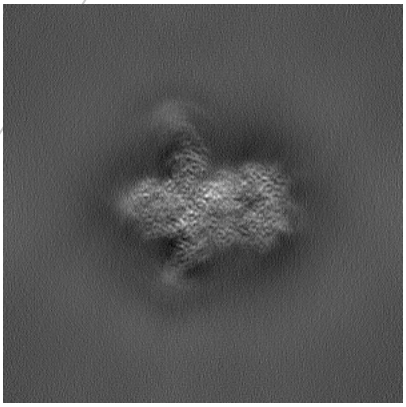


Z

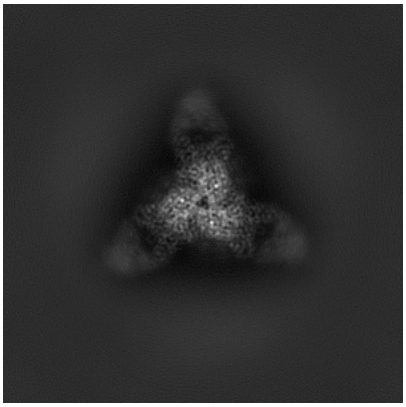
6.1.2 Raw map



X



Y

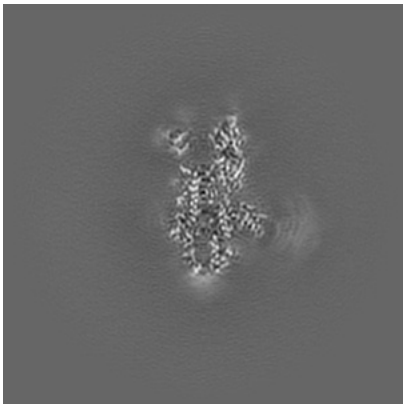


Z

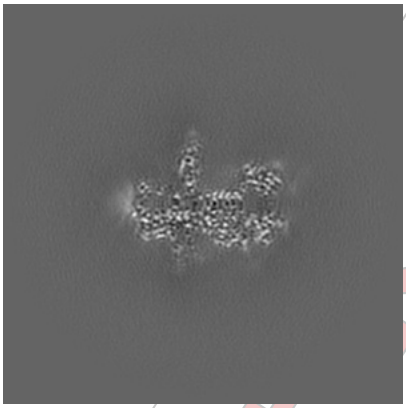
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

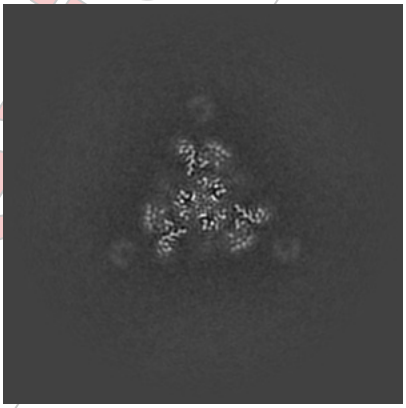
6.2.1 Primary map



X Index: 220

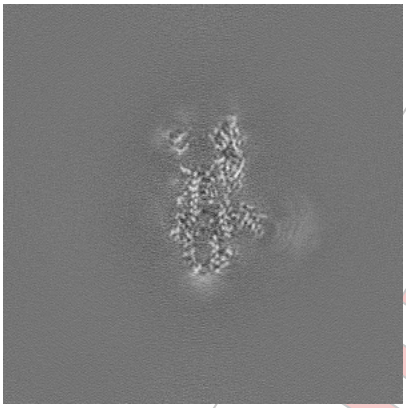


Y Index: 220

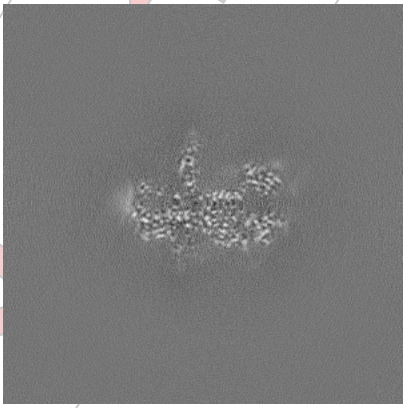


Z Index: 220

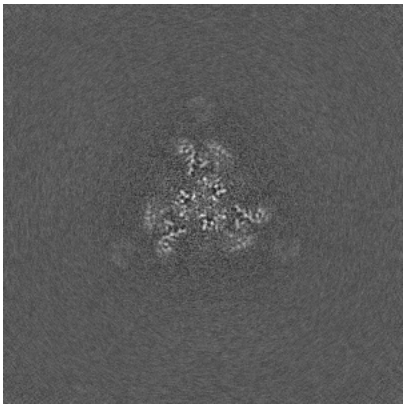
6.2.2 Raw map



X Index: 220



Y Index: 220

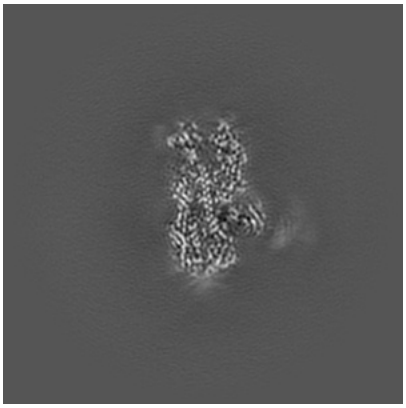


Z Index: 220

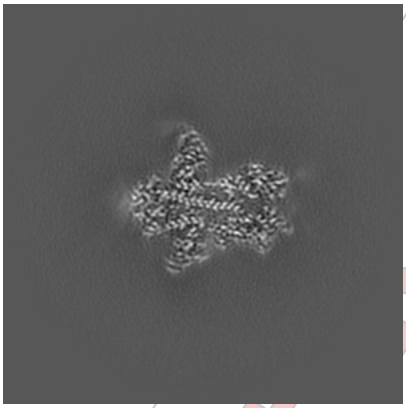
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

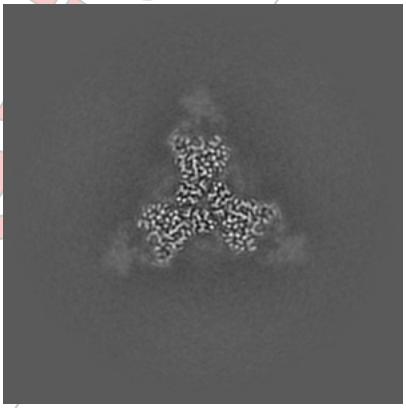
6.3.1 Primary map



X Index: 229

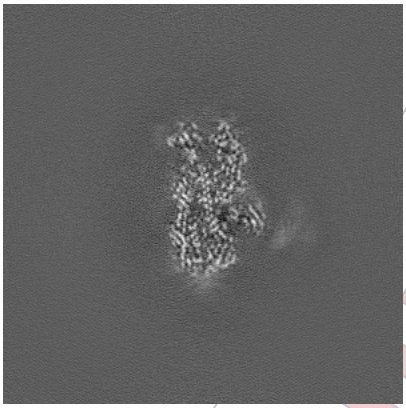


Y Index: 210

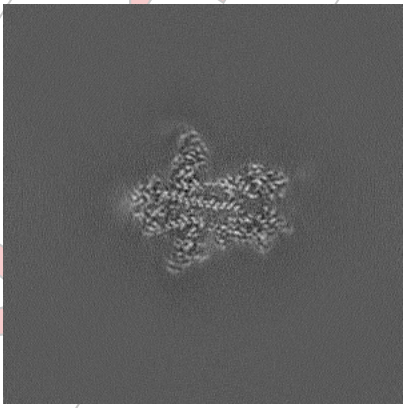


Z Index: 207

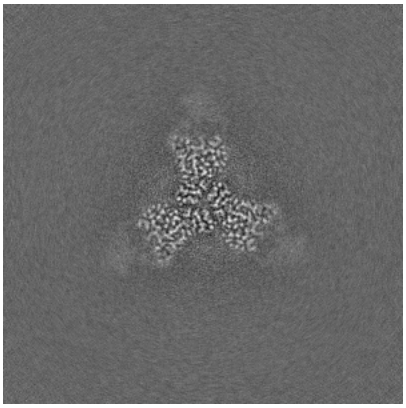
6.3.2 Raw map



X Index: 229



Y Index: 210

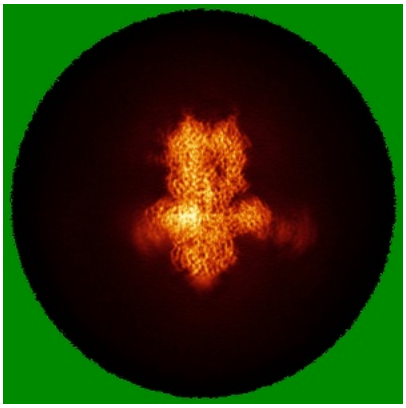


Z Index: 207

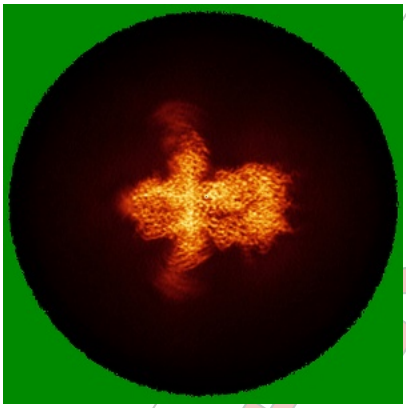
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

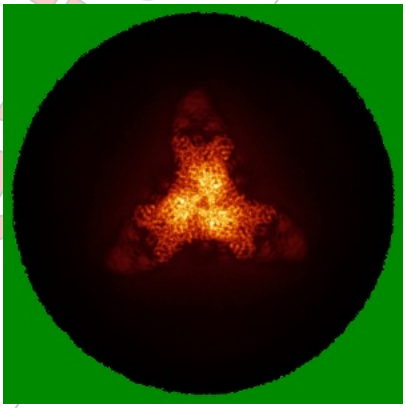
6.4.1 Primary map



X

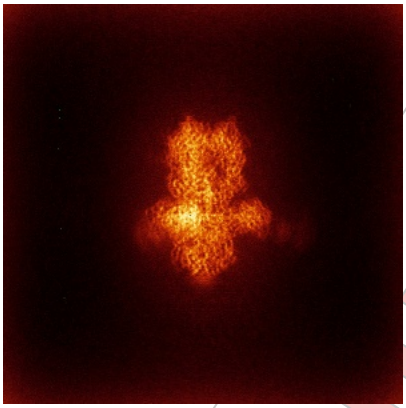


Y

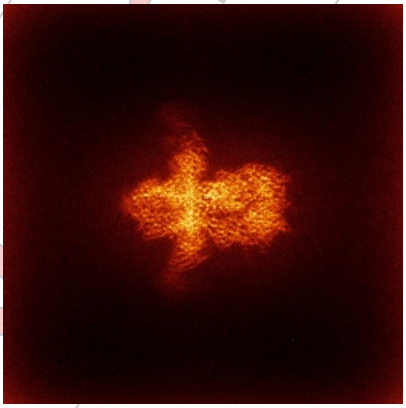


Z

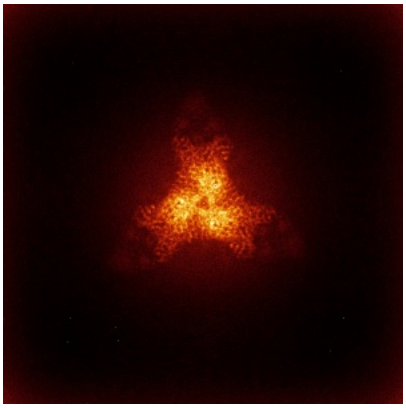
6.4.2 Raw map



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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

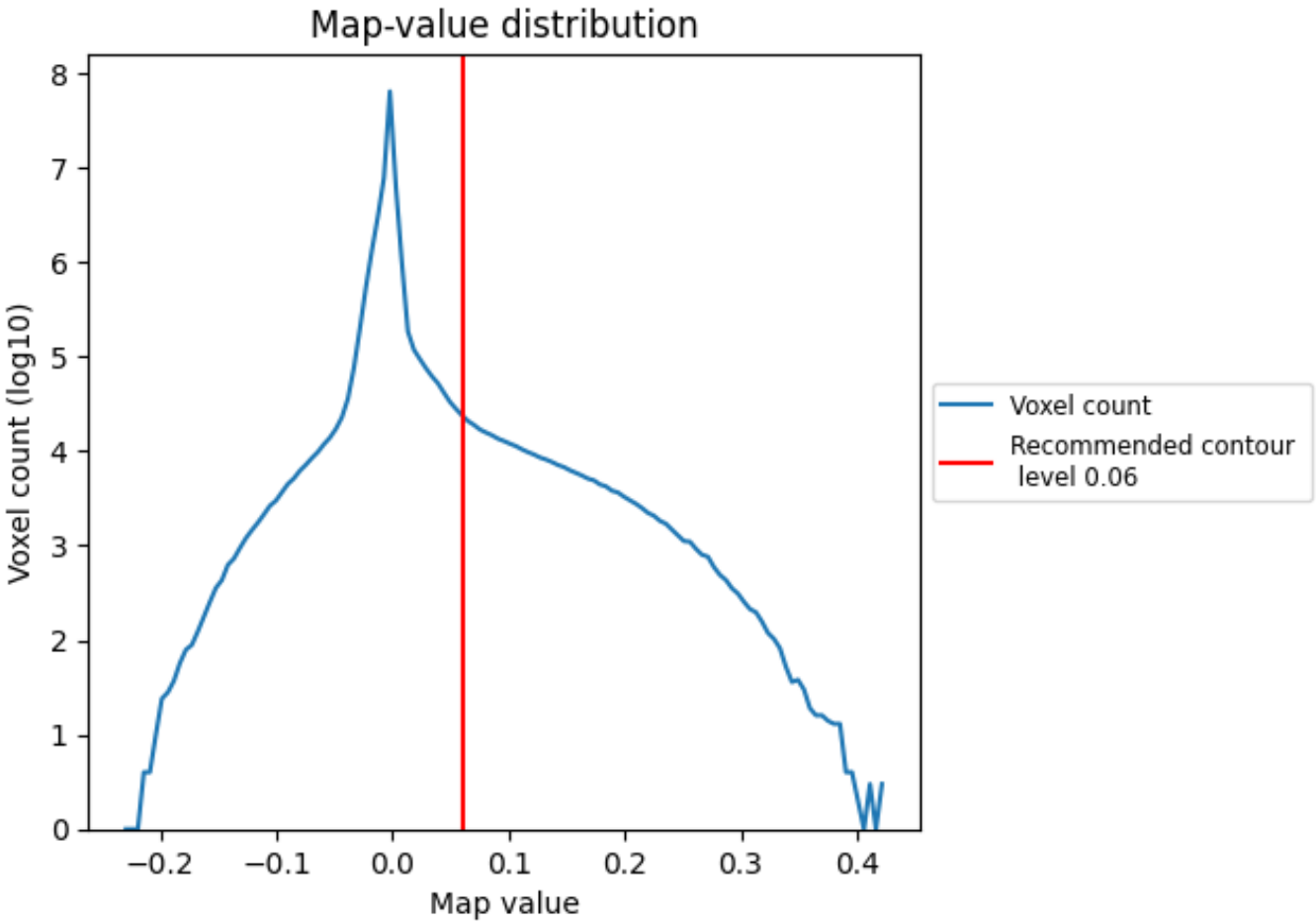
6.6 Mask visualisation (i)

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

7 Map analysis

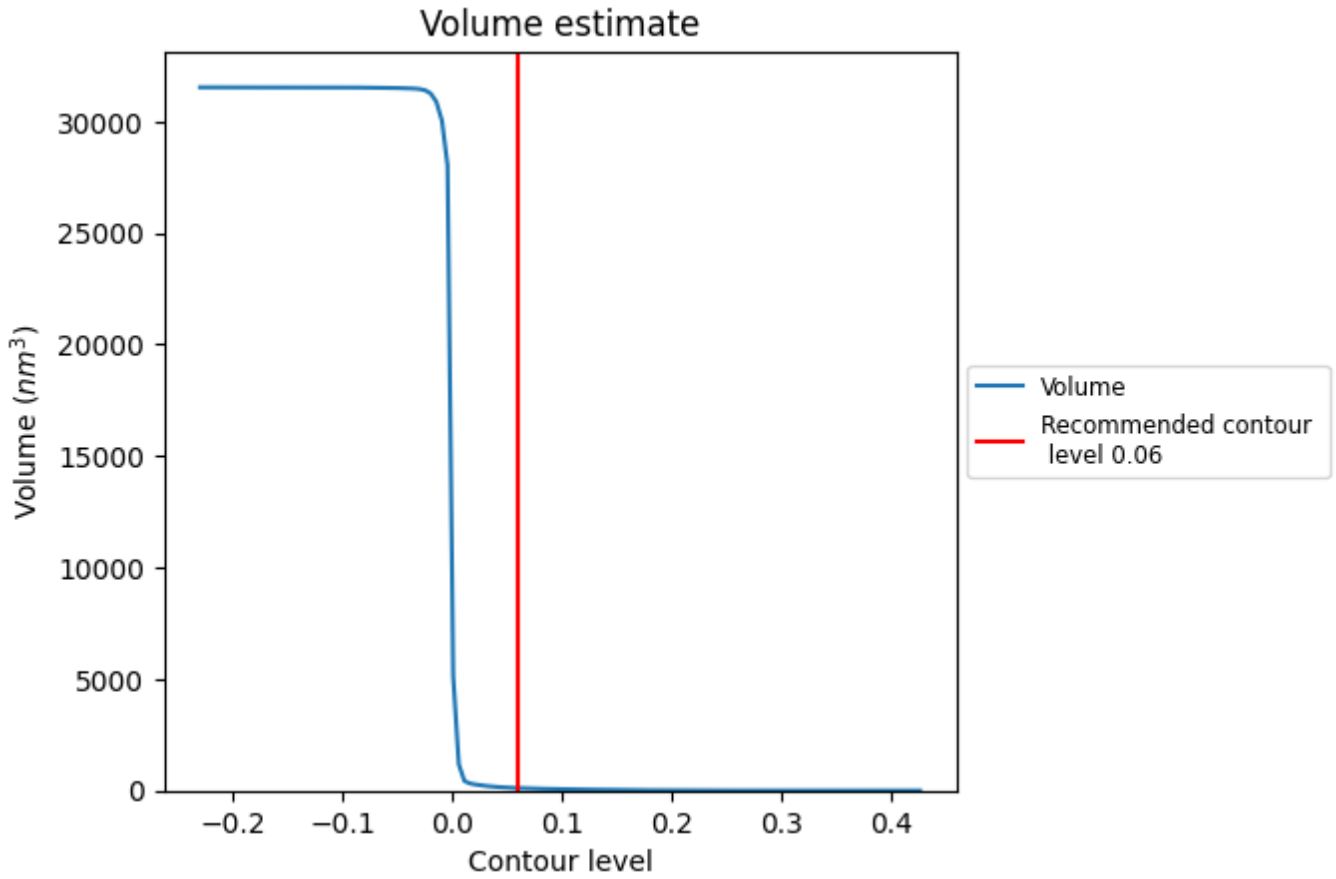
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

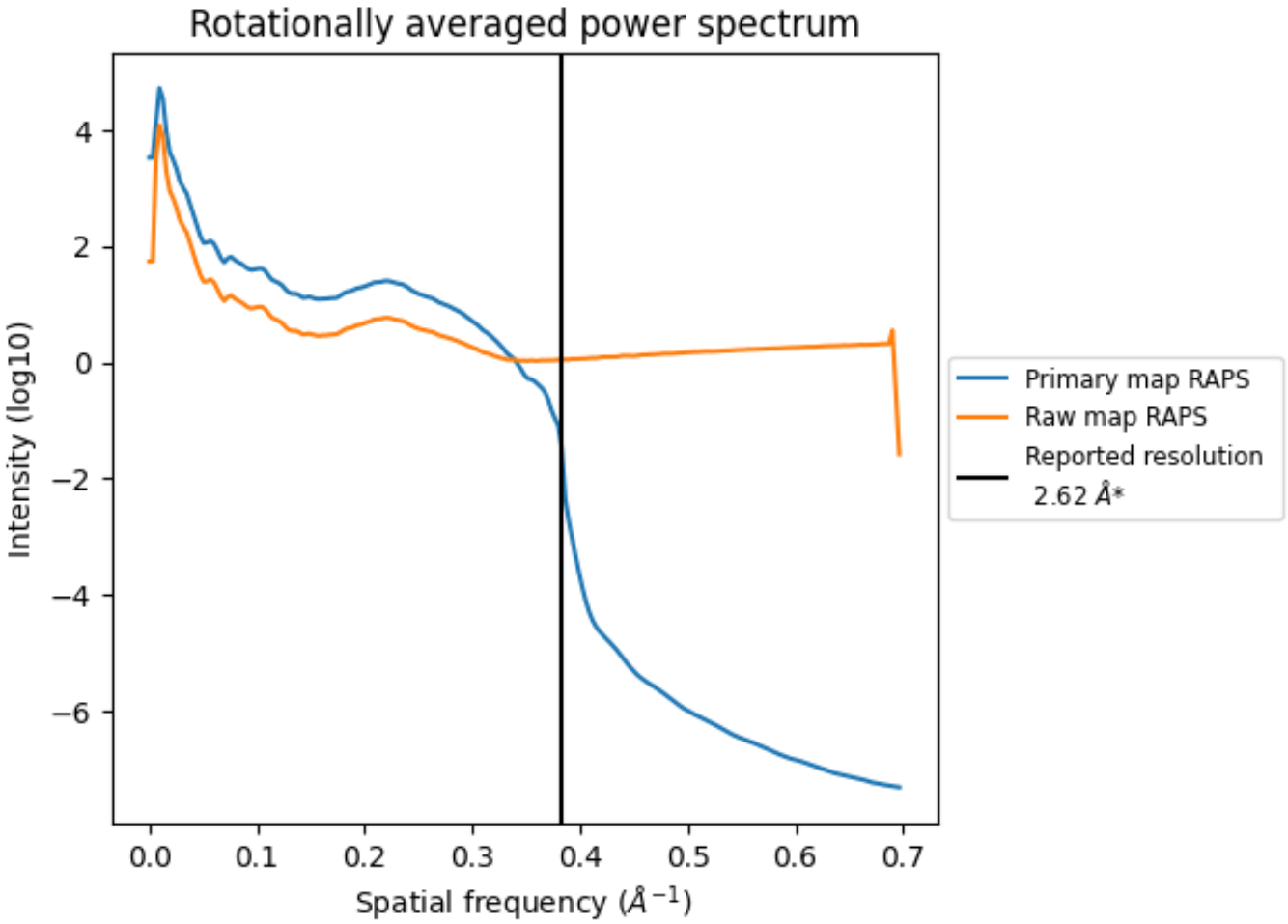
7.2 Volume estimate



The volume at the recommended contour level is 112 nm^3; this corresponds to an approximate mass of 101 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)

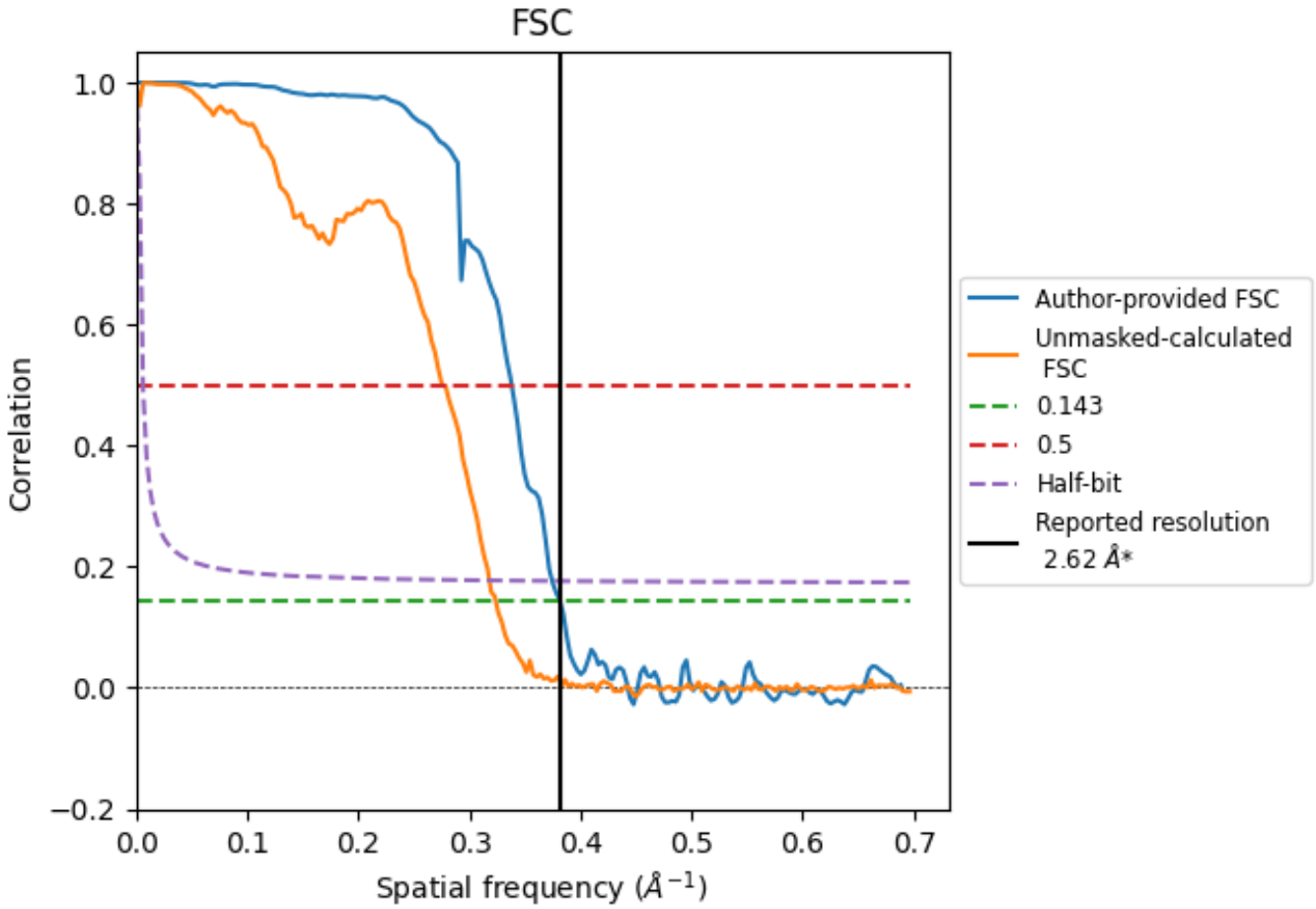


*Reported resolution corresponds to spatial frequency of 0.382 Å^{-1}

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 0.382 Å^{-1}

8.2 Resolution estimates (i)

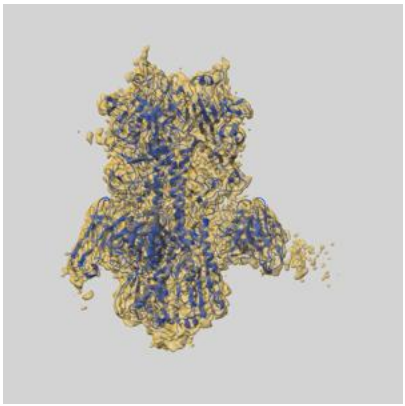
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	2.96	2.67
Unmasked-calculated*	3.09	3.61	3.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.62 by more than 10 %

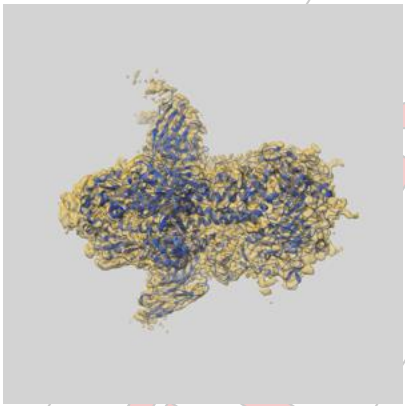
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70233 and PDB model 9O8Q. Per-residue inclusion information can be found in section 3 on page 12.

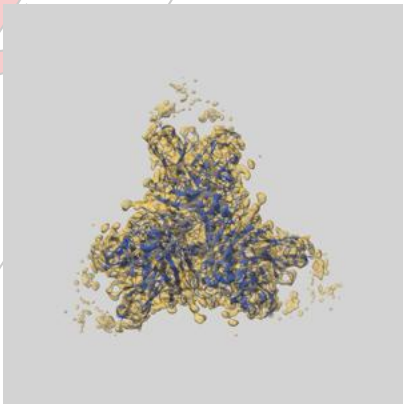
9.1 Map-model overlay



X



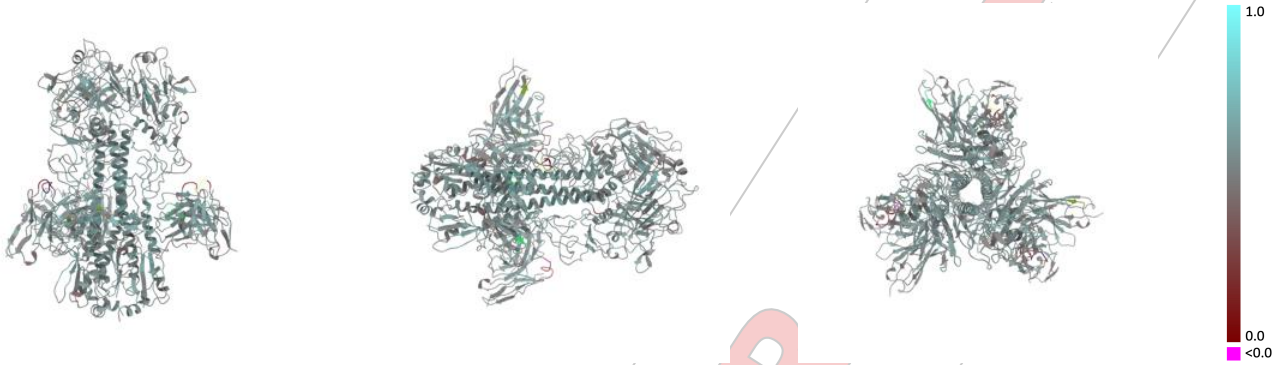
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

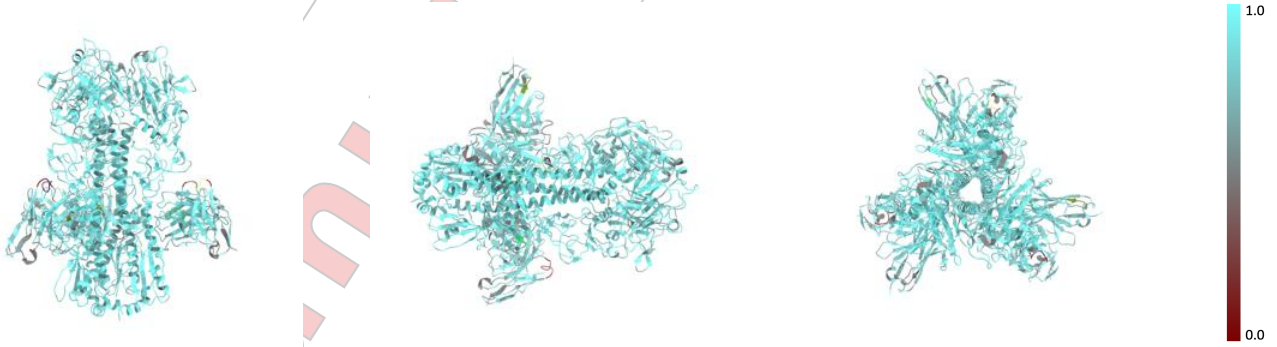
9.2 Q-score mapped to coordinate model



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.

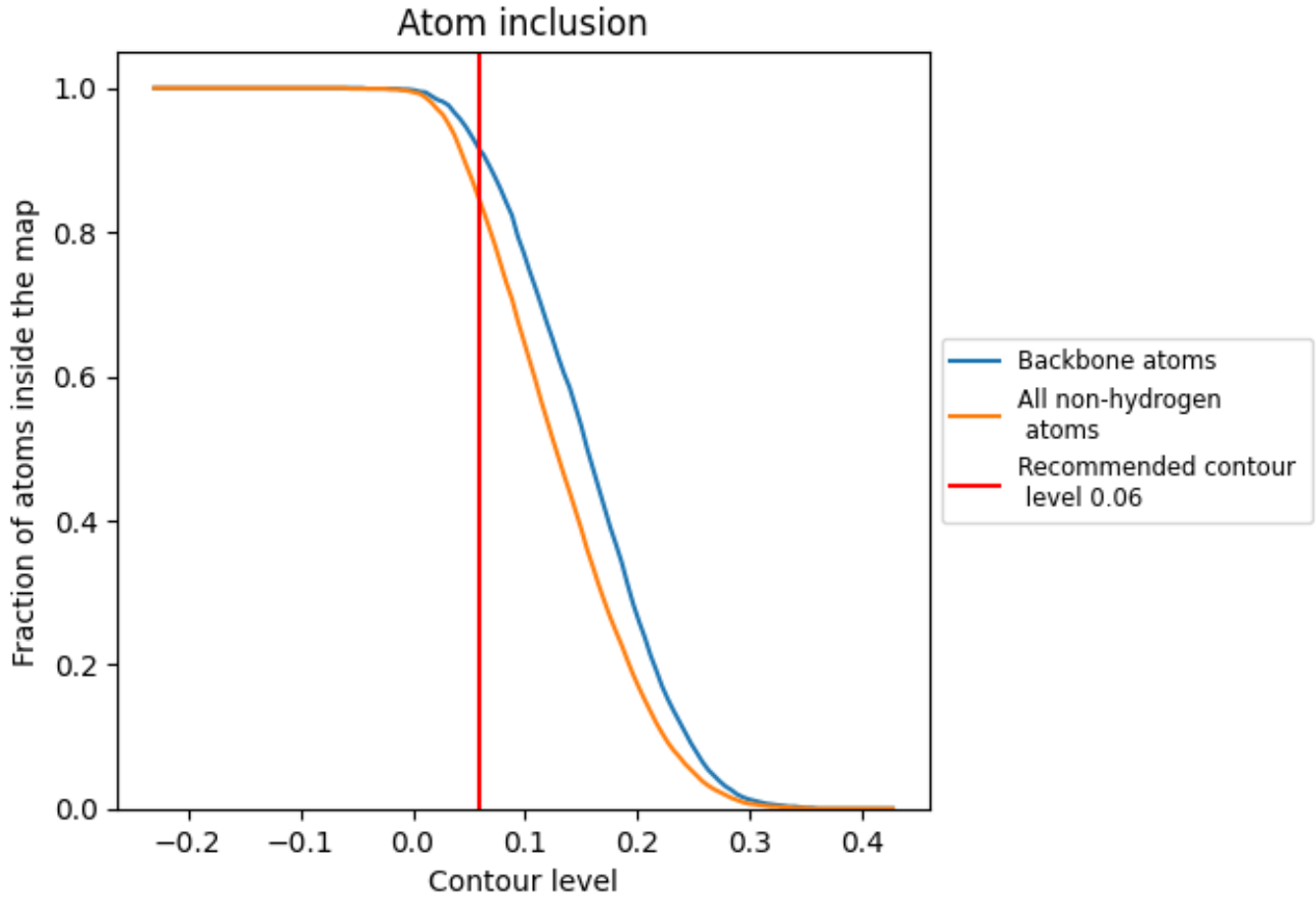
9.3 Atom inclusion mapped to coordinate model



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.5380
A	0.8550	0.5380
B	0.8940	0.5640
C	0.8560	0.5350
D	0.8590	0.5360
E	0.8930	0.5620
F	0.8900	0.5620
G	0.8500	0.5490
H	0.8450	0.5480
I	0.8440	0.5490
J	0.7500	0.5020
K	0.7510	0.4950
L	0.7500	0.4980
M	0.3080	0.5100
N	0.5530	0.4120
O	0.6410	0.5150
P	0.8460	0.4920
Q	0.3080	0.5230
R	0.5260	0.4120
S	0.6410	0.5120
T	0.8460	0.4970
U	0.3080	0.5180
V	0.5260	0.4060
W	0.6150	0.5030
X	0.8460	0.4980

Full wwPDB EM Validation Report (i)

Apr 17, 2025 – 01:24 PM EDT

PDB ID	:	9O8R / pdb_00009o8r
EMDB ID	:	EMD-70234
Title	:	Cryo-EM structure of NI06063_d30_103 Fab in complex with influenza virus hemagglutinin from A/Michigan/45/2015 (H1N1)
Deposited on	:	2025-04-16
Resolution	:	2.96 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (1)) were used in the production of this report:

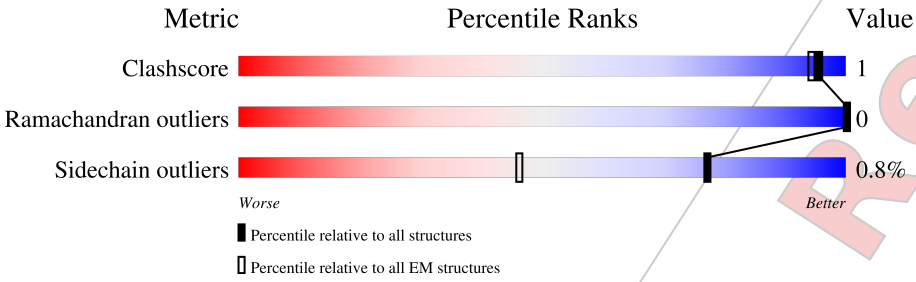
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.96 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	344	90% · 6%
1	C	344	90% · 6%
1	D	344	90% · 6%
2	B	233	71% · 28%
2	E	233	71% · 28%
2	F	233	71% · 28%
3	G	121	97% ·

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Mol	Chain	Length	Quality of chain
3	H	121	97%
3	I	121	97%
4	J	109	9% 96%
4	K	109	9% 94%
4	L	109	9% 96%
5	M	2	50% 50%
5	N	2	50% 50%
5	O	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17109 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	C	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	D	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	167	Total	C	N	O	S	0	0
			1355	849	232	268	6		
2	E	167	Total	C	N	O	S	0	0
			1355	849	232	268	6		
2	F	167	Total	C	N	O	S	0	0
			1355	849	232	268	6		

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	GLY	-	expression tag	UNP A0A1J0CXU0
B	177	TYR	-	expression tag	UNP A0A1J0CXU0
B	178	ILE	-	expression tag	UNP A0A1J0CXU0
B	179	PRO	-	expression tag	UNP A0A1J0CXU0
B	180	GLU	-	expression tag	UNP A0A1J0CXU0
B	181	ALA	-	expression tag	UNP A0A1J0CXU0
B	182	PRO	-	expression tag	UNP A0A1J0CXU0
B	183	ARG	-	expression tag	UNP A0A1J0CXU0
B	184	ASP	-	expression tag	UNP A0A1J0CXU0
B	185	GLY	-	expression tag	UNP A0A1J0CXU0
B	186	GLN	-	expression tag	UNP A0A1J0CXU0
B	187	ALA	-	expression tag	UNP A0A1J0CXU0
B	188	TYR	-	expression tag	UNP A0A1J0CXU0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	189	VAL	-	expression tag	UNP A0A1J0CXU0
B	190	ARG	-	expression tag	UNP A0A1J0CXU0
B	191	LYS	-	expression tag	UNP A0A1J0CXU0
B	192	ASP	-	expression tag	UNP A0A1J0CXU0
B	193	GLY	-	expression tag	UNP A0A1J0CXU0
B	194	GLU	-	expression tag	UNP A0A1J0CXU0
B	195	TRP	-	expression tag	UNP A0A1J0CXU0
B	196	VAL	-	expression tag	UNP A0A1J0CXU0
B	197	LEU	-	expression tag	UNP A0A1J0CXU0
B	198	LEU	-	expression tag	UNP A0A1J0CXU0
B	199	SER	-	expression tag	UNP A0A1J0CXU0
B	200	THR	-	expression tag	UNP A0A1J0CXU0
B	201	PHE	-	expression tag	UNP A0A1J0CXU0
B	202	LEU	-	expression tag	UNP A0A1J0CXU0
B	203	GLY	-	expression tag	UNP A0A1J0CXU0
B	204	SER	-	expression tag	UNP A0A1J0CXU0
B	205	GLU	-	expression tag	UNP A0A1J0CXU0
B	206	ASN	-	expression tag	UNP A0A1J0CXU0
B	207	LEU	-	expression tag	UNP A0A1J0CXU0
B	208	TYR	-	expression tag	UNP A0A1J0CXU0
B	209	PHE	-	expression tag	UNP A0A1J0CXU0
B	210	GLN	-	expression tag	UNP A0A1J0CXU0
B	211	GLY	-	expression tag	UNP A0A1J0CXU0
B	212	SER	-	expression tag	UNP A0A1J0CXU0
B	213	HIS	-	expression tag	UNP A0A1J0CXU0
B	214	HIS	-	expression tag	UNP A0A1J0CXU0
B	215	HIS	-	expression tag	UNP A0A1J0CXU0
B	216	HIS	-	expression tag	UNP A0A1J0CXU0
B	217	HIS	-	expression tag	UNP A0A1J0CXU0
B	218	HIS	-	expression tag	UNP A0A1J0CXU0
B	219	GLY	-	expression tag	UNP A0A1J0CXU0
B	220	LEU	-	expression tag	UNP A0A1J0CXU0
B	221	ASN	-	expression tag	UNP A0A1J0CXU0
B	222	ASP	-	expression tag	UNP A0A1J0CXU0
B	223	ILE	-	expression tag	UNP A0A1J0CXU0
B	224	PHE	-	expression tag	UNP A0A1J0CXU0
B	225	GLU	-	expression tag	UNP A0A1J0CXU0
B	226	ALA	-	expression tag	UNP A0A1J0CXU0
B	227	GLN	-	expression tag	UNP A0A1J0CXU0
B	228	LYS	-	expression tag	UNP A0A1J0CXU0
B	229	ILE	-	expression tag	UNP A0A1J0CXU0
B	230	GLU	-	expression tag	UNP A0A1J0CXU0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	TRP	-	expression tag	UNP A0A1J0CXU0
B	232	HIS	-	expression tag	UNP A0A1J0CXU0
B	233	GLU	-	expression tag	UNP A0A1J0CXU0
E	176	GLY	-	expression tag	UNP A0A1J0CXU0
E	177	TYR	-	expression tag	UNP A0A1J0CXU0
E	178	ILE	-	expression tag	UNP A0A1J0CXU0
E	179	PRO	-	expression tag	UNP A0A1J0CXU0
E	180	GLU	-	expression tag	UNP A0A1J0CXU0
E	181	ALA	-	expression tag	UNP A0A1J0CXU0
E	182	PRO	-	expression tag	UNP A0A1J0CXU0
E	183	ARG	-	expression tag	UNP A0A1J0CXU0
E	184	ASP	-	expression tag	UNP A0A1J0CXU0
E	185	GLY	-	expression tag	UNP A0A1J0CXU0
E	186	GLN	-	expression tag	UNP A0A1J0CXU0
E	187	ALA	-	expression tag	UNP A0A1J0CXU0
E	188	TYR	-	expression tag	UNP A0A1J0CXU0
E	189	VAL	-	expression tag	UNP A0A1J0CXU0
E	190	ARG	-	expression tag	UNP A0A1J0CXU0
E	191	LYS	-	expression tag	UNP A0A1J0CXU0
E	192	ASP	-	expression tag	UNP A0A1J0CXU0
E	193	GLY	-	expression tag	UNP A0A1J0CXU0
E	194	GLU	-	expression tag	UNP A0A1J0CXU0
E	195	TRP	-	expression tag	UNP A0A1J0CXU0
E	196	VAL	-	expression tag	UNP A0A1J0CXU0
E	197	LEU	-	expression tag	UNP A0A1J0CXU0
E	198	LEU	-	expression tag	UNP A0A1J0CXU0
E	199	SER	-	expression tag	UNP A0A1J0CXU0
E	200	THR	-	expression tag	UNP A0A1J0CXU0
E	201	PHE	-	expression tag	UNP A0A1J0CXU0
E	202	LEU	-	expression tag	UNP A0A1J0CXU0
E	203	GLY	-	expression tag	UNP A0A1J0CXU0
E	204	SER	-	expression tag	UNP A0A1J0CXU0
E	205	GLU	-	expression tag	UNP A0A1J0CXU0
E	206	ASN	-	expression tag	UNP A0A1J0CXU0
E	207	LEU	-	expression tag	UNP A0A1J0CXU0
E	208	TYR	-	expression tag	UNP A0A1J0CXU0
E	209	PHE	-	expression tag	UNP A0A1J0CXU0
E	210	GLN	-	expression tag	UNP A0A1J0CXU0
E	211	GLY	-	expression tag	UNP A0A1J0CXU0
E	212	SER	-	expression tag	UNP A0A1J0CXU0
E	213	HIS	-	expression tag	UNP A0A1J0CXU0
E	214	HIS	-	expression tag	UNP A0A1J0CXU0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	215	HIS	-	expression tag	UNP A0A1J0CXU0
E	216	HIS	-	expression tag	UNP A0A1J0CXU0
E	217	HIS	-	expression tag	UNP A0A1J0CXU0
E	218	HIS	-	expression tag	UNP A0A1J0CXU0
E	219	GLY	-	expression tag	UNP A0A1J0CXU0
E	220	LEU	-	expression tag	UNP A0A1J0CXU0
E	221	ASN	-	expression tag	UNP A0A1J0CXU0
E	222	ASP	-	expression tag	UNP A0A1J0CXU0
E	223	ILE	-	expression tag	UNP A0A1J0CXU0
E	224	PHE	-	expression tag	UNP A0A1J0CXU0
E	225	GLU	-	expression tag	UNP A0A1J0CXU0
E	226	ALA	-	expression tag	UNP A0A1J0CXU0
E	227	GLN	-	expression tag	UNP A0A1J0CXU0
E	228	LYS	-	expression tag	UNP A0A1J0CXU0
E	229	ILE	-	expression tag	UNP A0A1J0CXU0
E	230	GLU	-	expression tag	UNP A0A1J0CXU0
E	231	TRP	-	expression tag	UNP A0A1J0CXU0
E	232	HIS	-	expression tag	UNP A0A1J0CXU0
E	233	GLU	-	expression tag	UNP A0A1J0CXU0
F	176	GLY	-	expression tag	UNP A0A1J0CXU0
F	177	TYR	-	expression tag	UNP A0A1J0CXU0
F	178	ILE	-	expression tag	UNP A0A1J0CXU0
F	179	PRO	-	expression tag	UNP A0A1J0CXU0
F	180	GLU	-	expression tag	UNP A0A1J0CXU0
F	181	ALA	-	expression tag	UNP A0A1J0CXU0
F	182	PRO	-	expression tag	UNP A0A1J0CXU0
F	183	ARG	-	expression tag	UNP A0A1J0CXU0
F	184	ASP	-	expression tag	UNP A0A1J0CXU0
F	185	GLY	-	expression tag	UNP A0A1J0CXU0
F	186	GLN	-	expression tag	UNP A0A1J0CXU0
F	187	ALA	-	expression tag	UNP A0A1J0CXU0
F	188	TYR	-	expression tag	UNP A0A1J0CXU0
F	189	VAL	-	expression tag	UNP A0A1J0CXU0
F	190	ARG	-	expression tag	UNP A0A1J0CXU0
F	191	LYS	-	expression tag	UNP A0A1J0CXU0
F	192	ASP	-	expression tag	UNP A0A1J0CXU0
F	193	GLY	-	expression tag	UNP A0A1J0CXU0
F	194	GLU	-	expression tag	UNP A0A1J0CXU0
F	195	TRP	-	expression tag	UNP A0A1J0CXU0
F	196	VAL	-	expression tag	UNP A0A1J0CXU0
F	197	LEU	-	expression tag	UNP A0A1J0CXU0
F	198	LEU	-	expression tag	UNP A0A1J0CXU0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	199	SER	-	expression tag	UNP A0A1J0CXU0
F	200	THR	-	expression tag	UNP A0A1J0CXU0
F	201	PHE	-	expression tag	UNP A0A1J0CXU0
F	202	LEU	-	expression tag	UNP A0A1J0CXU0
F	203	GLY	-	expression tag	UNP A0A1J0CXU0
F	204	SER	-	expression tag	UNP A0A1J0CXU0
F	205	GLU	-	expression tag	UNP A0A1J0CXU0
F	206	ASN	-	expression tag	UNP A0A1J0CXU0
F	207	LEU	-	expression tag	UNP A0A1J0CXU0
F	208	TYR	-	expression tag	UNP A0A1J0CXU0
F	209	PHE	-	expression tag	UNP A0A1J0CXU0
F	210	GLN	-	expression tag	UNP A0A1J0CXU0
F	211	GLY	-	expression tag	UNP A0A1J0CXU0
F	212	SER	-	expression tag	UNP A0A1J0CXU0
F	213	HIS	-	expression tag	UNP A0A1J0CXU0
F	214	HIS	-	expression tag	UNP A0A1J0CXU0
F	215	HIS	-	expression tag	UNP A0A1J0CXU0
F	216	HIS	-	expression tag	UNP A0A1J0CXU0
F	217	HIS	-	expression tag	UNP A0A1J0CXU0
F	218	HIS	-	expression tag	UNP A0A1J0CXU0
F	219	GLY	-	expression tag	UNP A0A1J0CXU0
F	220	LEU	-	expression tag	UNP A0A1J0CXU0
F	221	ASN	-	expression tag	UNP A0A1J0CXU0
F	222	ASP	-	expression tag	UNP A0A1J0CXU0
F	223	ILE	-	expression tag	UNP A0A1J0CXU0
F	224	PHE	-	expression tag	UNP A0A1J0CXU0
F	225	GLU	-	expression tag	UNP A0A1J0CXU0
F	226	ALA	-	expression tag	UNP A0A1J0CXU0
F	227	GLN	-	expression tag	UNP A0A1J0CXU0
F	228	LYS	-	expression tag	UNP A0A1J0CXU0
F	229	ILE	-	expression tag	UNP A0A1J0CXU0
F	230	GLU	-	expression tag	UNP A0A1J0CXU0
F	231	TRP	-	expression tag	UNP A0A1J0CXU0
F	232	HIS	-	expression tag	UNP A0A1J0CXU0
F	233	GLU	-	expression tag	UNP A0A1J0CXU0

- Molecule 3 is a protein called NI06063_d30_103 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			951	605	163	178	5		
3	G	121	Total	C	N	O	S	0	0
			951	605	163	178	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	121	Total 951	C 605	N 163	O 178	S 5	0	0

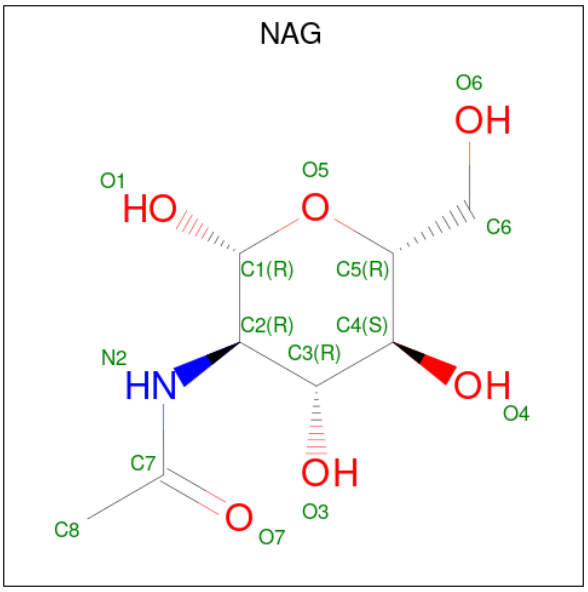
- Molecule 4 is a protein called NI06063_d30_103 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total 771	C 477	N 134	O 156	S 4	0	0
4	J	107	Total 771	C 477	N 134	O 156	S 4	0	0
4	K	107	Total 771	C 477	N 134	O 156	S 4	0	0

- Molecule 5 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
5	M	2	Total 28	C 16	N 2	O 10	0	0
5	N	2	Total 28	C 16	N 2	O 10	0	0
5	O	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

3 Residue-property plots (i)

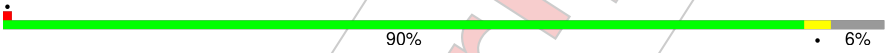
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

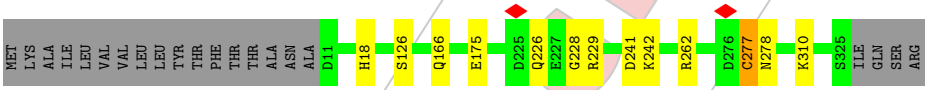
- Molecule 1: Hemagglutinin

Chain A:

- Molecule 1: Hemagglutinin

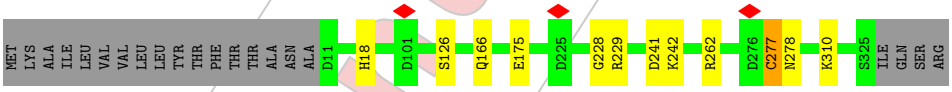
Chain C:





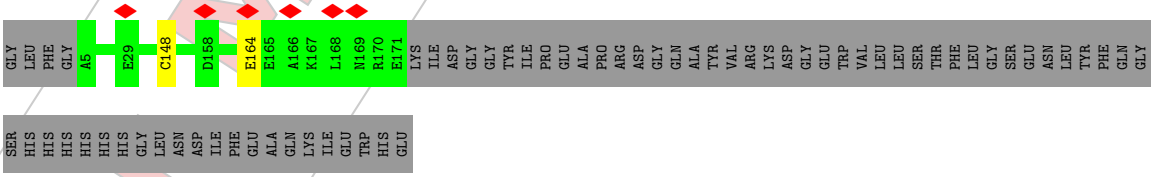
- Molecule 1: Hemagglutinin

Chain D:



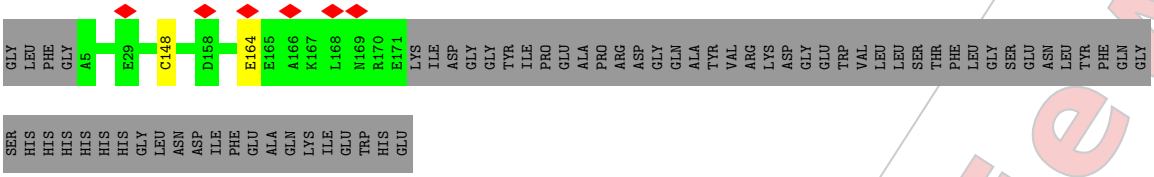
- Molecule 2: Hemagglutinin

Chain B:



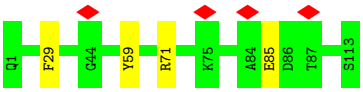
- Molecule 2: Hemagglutinin

Chain E:

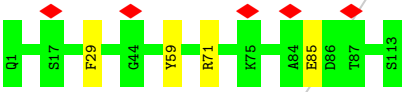


• Molecule 2: Hemagglutinin

• Molecule 3: NI06063_d30_103 Fab heavy chain

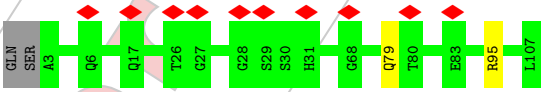


• Molecule 3: NI06063_d30_103 Fab heavy chain

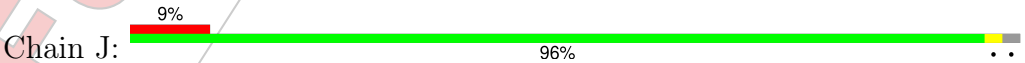


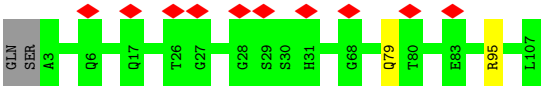
• Molecule 3: NI06063_d30_103 Fab heavy chain

• Molecule 4: NI06063_d30_103 Fab light chain



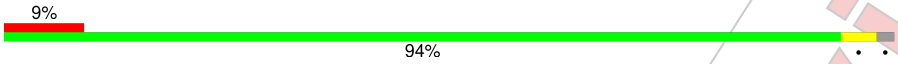
• Molecule 4: NI06063_d30_103 Fab light chain

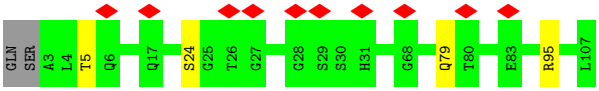




• Molecule 4: NI06063_d30_103 Fab light chain

Chain K:





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

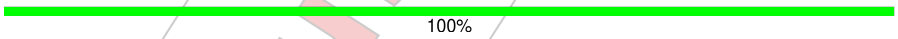
Chain M:

• 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 O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	276374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	44.87	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.030	Depositor
Minimum map value	-0.895	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	319.0, 319.0, 319.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/2591	0.55	0/3525
1	C	0.29	0/2591	0.55	0/3525
1	D	0.29	0/2591	0.55	0/3525
2	B	0.29	0/1382	0.52	0/1862
2	E	0.29	0/1382	0.52	0/1862
2	F	0.29	0/1382	0.52	0/1862
3	G	0.31	0/977	0.58	0/1322
3	H	0.31	0/977	0.58	0/1322
3	I	0.31	0/977	0.58	0/1322
4	J	0.30	0/787	0.61	0/1063
4	K	0.30	0/787	0.61	0/1063
4	L	0.30	0/787	0.61	0/1063
All	All	0.29	0/17211	0.55	0/23316

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2459	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2528	0	2459	6	0
1	D	2528	0	2459	5	0
2	B	1355	0	1281	1	0
2	E	1355	0	1281	1	0
2	F	1355	0	1281	1	0
3	G	951	0	893	3	0
3	H	951	0	893	3	0
3	I	951	0	893	3	0
4	J	771	0	747	1	0
4	K	771	0	747	2	0
4	L	771	0	747	1	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
6	A	56	0	52	0	0
6	B	14	0	13	0	0
6	C	56	0	52	0	0
6	D	56	0	52	0	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
All	All	17109	0	16410	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (31) 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)
3:H:59:TYR:O	4:L:95:ARG:NH2	2.26	0.69
3:I:59:TYR:O	4:K:95:ARG:NH2	2.26	0.69
3:G:59:TYR:O	4:J:95:ARG:NH2	2.26	0.68
1:D:175:GLU:OE1	1:D:262:ARG:NH1	2.38	0.56
1:A:175:GLU:OE1	1:A:262:ARG:NH1	2.40	0.55
1:C:175:GLU:OE1	1:C:262:ARG:NH1	2.39	0.54
2:E:164:GLU:N	2:E:164:GLU:OE1	2.40	0.54
2:F:164:GLU:N	2:F:164:GLU:OE1	2.40	0.54
2:B:164:GLU:N	2:B:164:GLU:OE1	2.40	0.54
3:G:29:PHE:O	3:G:71:ARG:NH2	2.42	0.53
3:I:29:PHE:O	3:I:71:ARG:NH2	2.42	0.52
1:A:126:SER:O	1:A:166:GLN:NE2	2.42	0.52
1:A:228:GLY:O	1:A:229:ARG:NE	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:29:PHE:O	3:H:71:ARG:NH2	2.43	0.52
1:C:126:SER:O	1:C:166:GLN:NE2	2.43	0.52
1:D:228:GLY:O	1:D:229:ARG:NE	2.42	0.51
1:D:126:SER:O	1:D:166:GLN:NE2	2.44	0.51
1:C:228:GLY:O	1:C:229:ARG:NE	2.42	0.51
1:C:277:CYS:SG	1:C:278:ASN:N	2.85	0.49
1:A:277:CYS:SG	1:A:278:ASN:N	2.85	0.49
1:D:277:CYS:SG	1:D:278:ASN:N	2.85	0.48
3:H:85:GLU:OE1	3:H:85:GLU:N	2.49	0.45
3:I:85:GLU:OE1	3:I:85:GLU:N	2.49	0.44
3:G:85:GLU:OE1	3:G:85:GLU:N	2.49	0.43
4:K:5:THR:N	4:K:24:SER:O	2.45	0.43
1:D:241:ASP:OD1	1:D:242:LYS:N	2.54	0.41
1:A:241:ASP:OD1	1:A:242:LYS:N	2.54	0.41
1:C:226:GLN:O	1:C:229:ARG:NH2	2.52	0.41
1:A:128:PRO:O	1:A:157:LYS:NZ	2.50	0.40
1:C:241:ASP:OD1	1:C:242:LYS:N	2.54	0.40
1:A:226:GLN:O	1:A:229:ARG:NH2	2.54	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	321/344 (93%)	314 (98%)	7 (2%)	0	100	100
1	C	321/344 (93%)	314 (98%)	7 (2%)	0	100	100
1	D	321/344 (93%)	315 (98%)	6 (2%)	0	100	100
2	B	165/233 (71%)	163 (99%)	2 (1%)	0	100	100
2	E	165/233 (71%)	163 (99%)	2 (1%)	0	100	100
2	F	165/233 (71%)	163 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
3	H	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
3	I	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
4	J	105/109 (96%)	98 (93%)	7 (7%)	0	100	100
4	K	105/109 (96%)	98 (93%)	7 (7%)	0	100	100
4	L	105/109 (96%)	98 (93%)	7 (7%)	0	100	100
All	All	2130/2421 (88%)	2062 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/302 (94%)	281 (99%)	3 (1%)	70	83
1	C	284/302 (94%)	281 (99%)	3 (1%)	70	83
1	D	284/302 (94%)	281 (99%)	3 (1%)	70	83
2	B	145/199 (73%)	144 (99%)	1 (1%)	81	90
2	E	145/199 (73%)	144 (99%)	1 (1%)	81	90
2	F	145/199 (73%)	144 (99%)	1 (1%)	81	90
3	G	97/98 (99%)	97 (100%)	0	100	100
3	H	97/98 (99%)	97 (100%)	0	100	100
3	I	97/98 (99%)	97 (100%)	0	100	100
4	J	85/87 (98%)	84 (99%)	1 (1%)	67	82
4	K	85/87 (98%)	84 (99%)	1 (1%)	67	82
4	L	85/87 (98%)	84 (99%)	1 (1%)	67	82
All	All	1833/2058 (89%)	1818 (99%)	15 (1%)	77	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	277	CYS
1	A	310	LYS
2	B	148	CYS
4	L	79	GLN
1	C	18	HIS
1	C	277	CYS
1	C	310	LYS
2	E	148	CYS
4	J	79	GLN
1	D	18	HIS
1	D	277	CYS
1	D	310	LYS
2	F	148	CYS
4	K	79	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 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	5,1	14,14,15	0.21	0	17,19,21	0.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	N	1	5,1	14,14,15	0.18	0	17,19,21	0.62	1 (5%)
5	NAG	N	2	5	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	O	1	5,1	14,14,15	0.19	0	17,19,21	0.61	0
5	NAG	O	2	5	14,14,15	0.24	0	17,19,21	0.43	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
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	1	NAG	C1-O5-C5	2.04	114.92	112.19
5	M	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
5	M	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6

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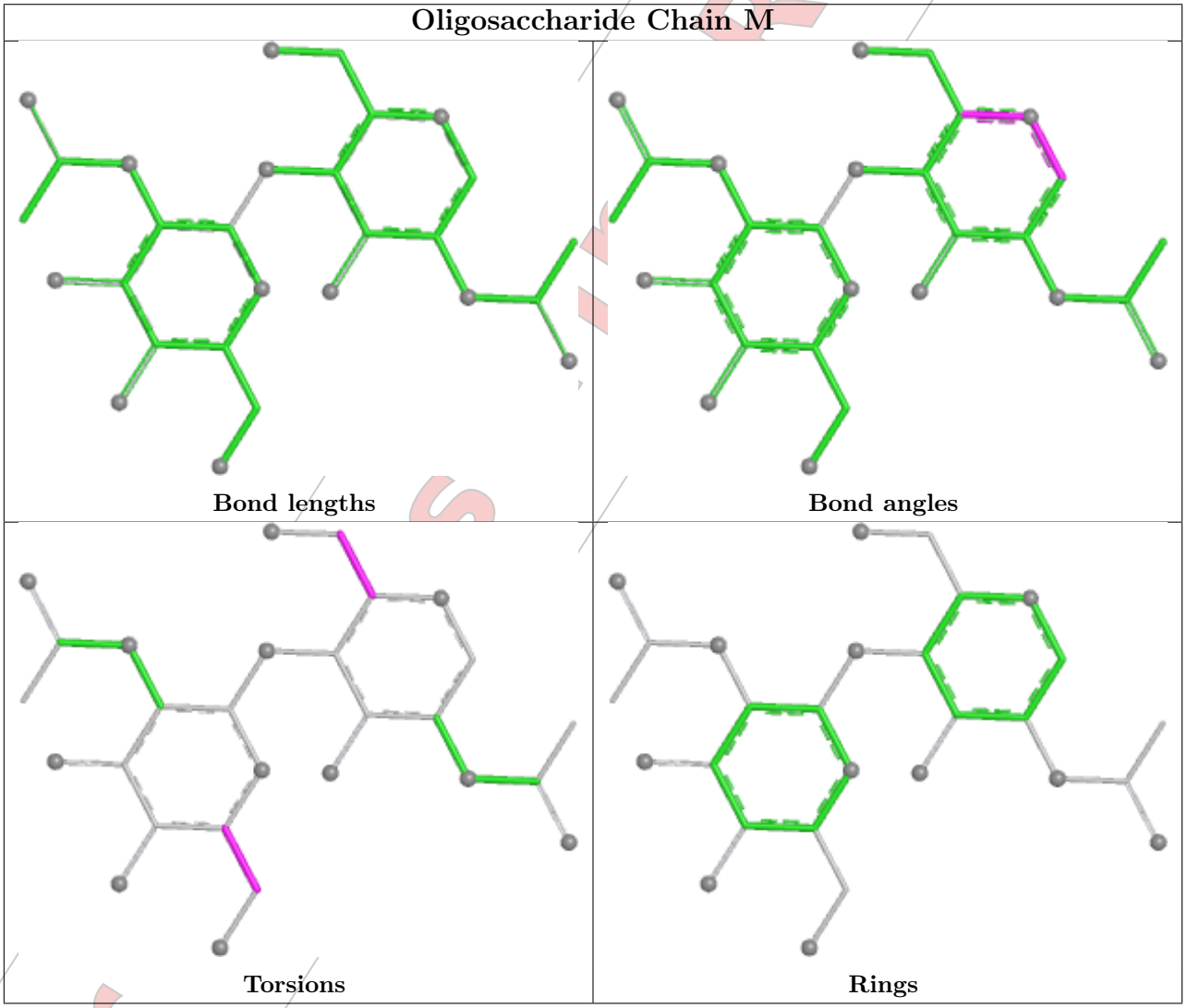
Mol	Chain	Res	Type	Atoms
5	N	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6

There are no ring outliers.

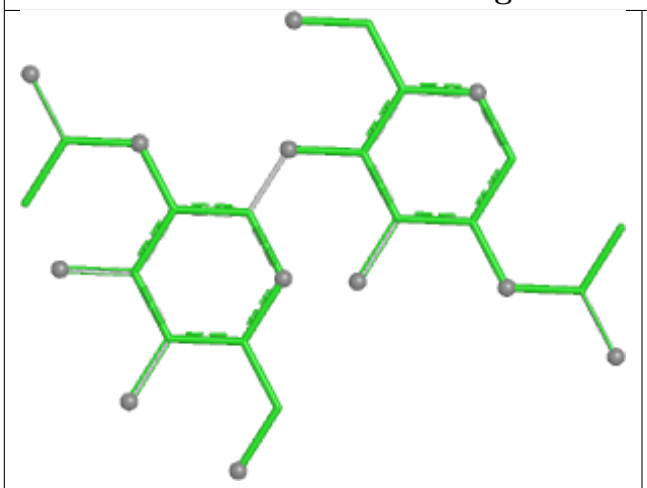
No monomer is involved in short contacts.

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

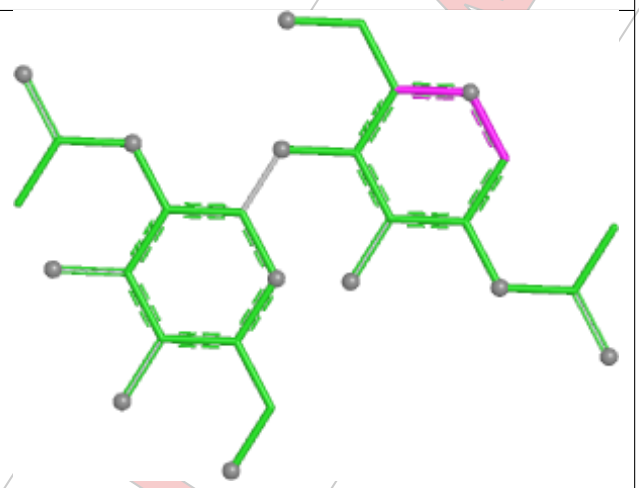
Oligosaccharide Chain M



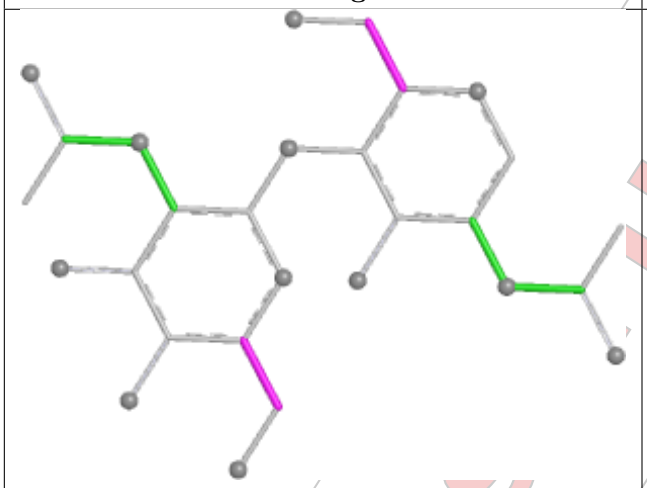
Oligosaccharide Chain N



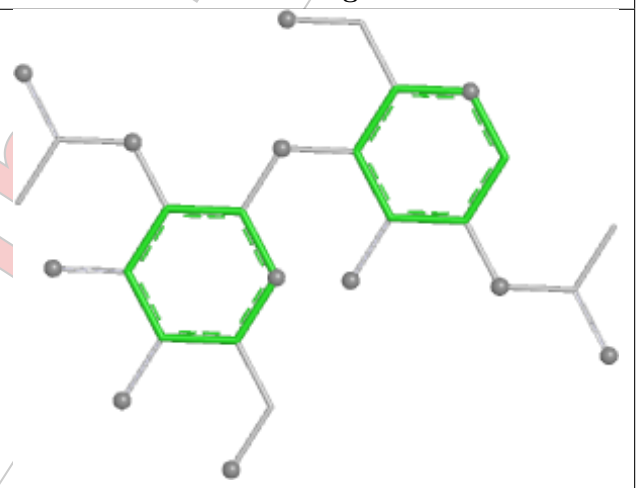
Bond lengths



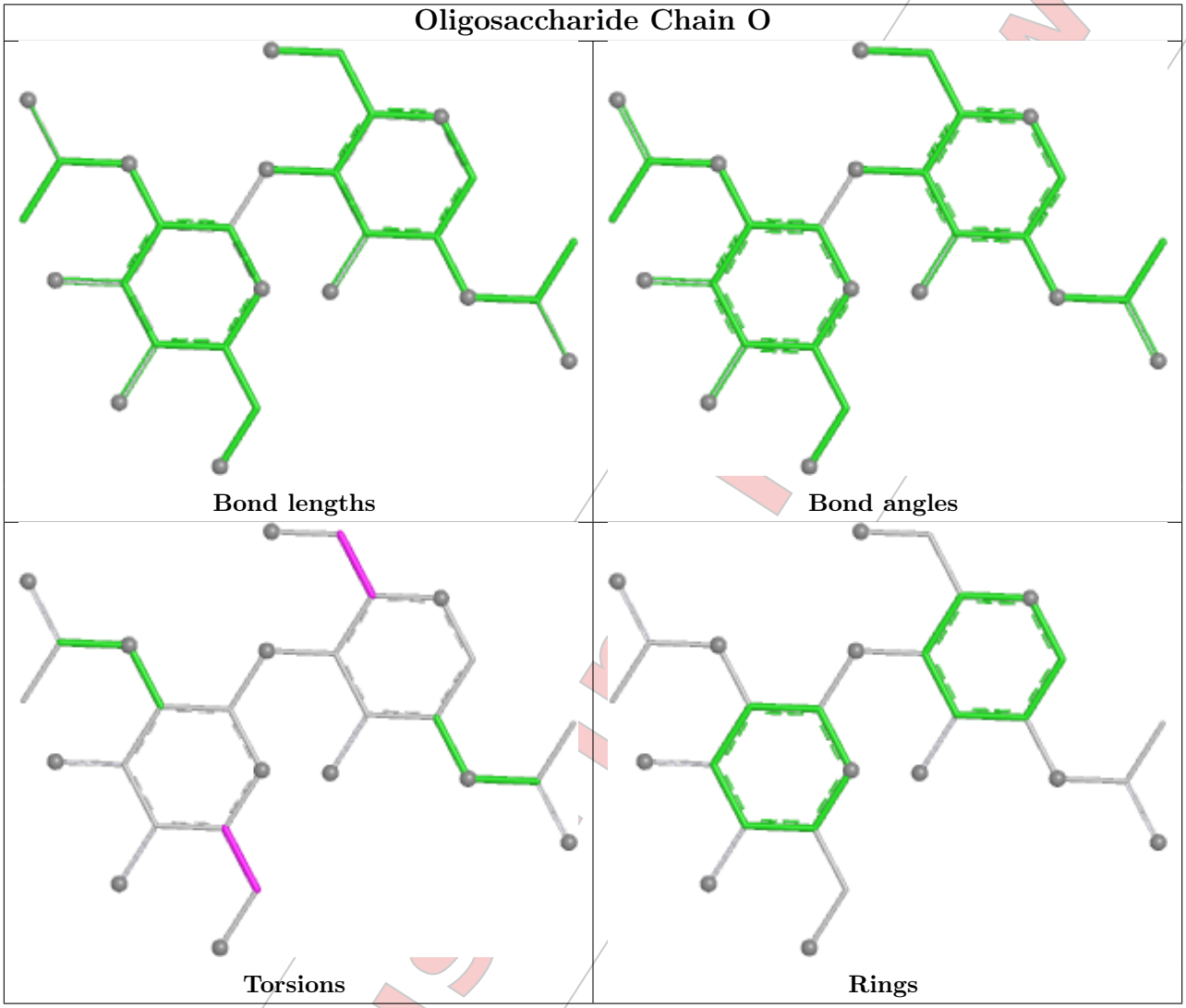
Bond angles



Torsions



Rings



5.6 Ligand geometry

15 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	$\#\|Z\| > 2$
6	NAG	C	402	1	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	A	401	1	14,14,15	0.18	0	17,19,21	0.43	0
6	NAG	A	402	1	14,14,15	0.24	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	C	401	1	14,14,15	0.18	0	17,19,21	0.42	0
6	NAG	D	401	1	14,14,15	0.17	0	17,19,21	0.43	0
6	NAG	D	402	1	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	A	403	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	E	301	2	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	D	403	1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	B	301	2	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	F	301	2	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	C	403	1	14,14,15	0.19	0	17,19,21	0.42	0
6	NAG	A	404	1	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	C	404	1	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	D	404	1	14,14,15	0.24	0	17,19,21	0.46	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	C	402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	402	1	-	2/6/23/26	0/1/1/1
6	NAG	C	401	1	-	2/6/23/26	0/1/1/1
6	NAG	D	401	1	-	2/6/23/26	0/1/1/1
6	NAG	D	402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	403	1	-	1/6/23/26	0/1/1/1
6	NAG	E	301	2	-	1/6/23/26	0/1/1/1
6	NAG	D	403	1	-	1/6/23/26	0/1/1/1
6	NAG	B	301	2	-	1/6/23/26	0/1/1/1
6	NAG	F	301	2	-	1/6/23/26	0/1/1/1
6	NAG	C	403	1	-	1/6/23/26	0/1/1/1
6	NAG	A	404	1	-	2/6/23/26	0/1/1/1
6	NAG	C	404	1	-	2/6/23/26	0/1/1/1
6	NAG	D	404	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	402	NAG	O5-C5-C6-O6
6	A	402	NAG	O5-C5-C6-O6
6	C	402	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	C	401	NAG	C4-C5-C6-O6
6	D	401	NAG	C4-C5-C6-O6
6	C	402	NAG	C4-C5-C6-O6
6	D	402	NAG	C4-C5-C6-O6
6	A	402	NAG	C4-C5-C6-O6
6	D	401	NAG	O5-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6
6	A	403	NAG	O5-C5-C6-O6
6	C	403	NAG	O5-C5-C6-O6
6	D	403	NAG	O5-C5-C6-O6
6	B	301	NAG	C4-C5-C6-O6
6	C	404	NAG	C4-C5-C6-O6
6	E	301	NAG	C4-C5-C6-O6
6	D	404	NAG	C4-C5-C6-O6
6	A	404	NAG	C4-C5-C6-O6
6	F	301	NAG	C4-C5-C6-O6
6	C	404	NAG	O5-C5-C6-O6
6	D	404	NAG	O5-C5-C6-O6
6	A	404	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

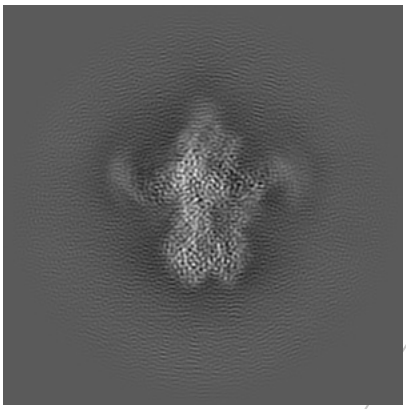
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70234. These allow visual inspection of the internal detail of the map and identification of artifacts.

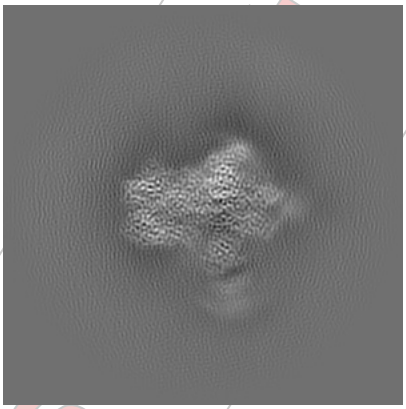
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

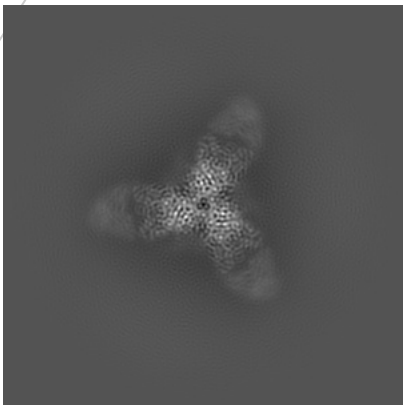
6.1.1 Primary map



X

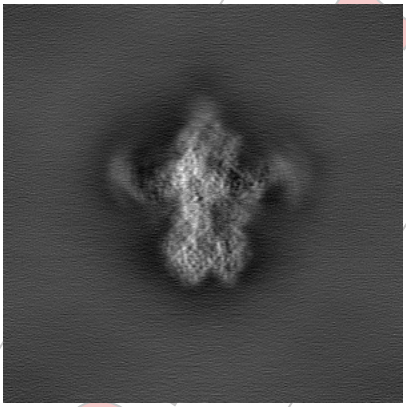


Y

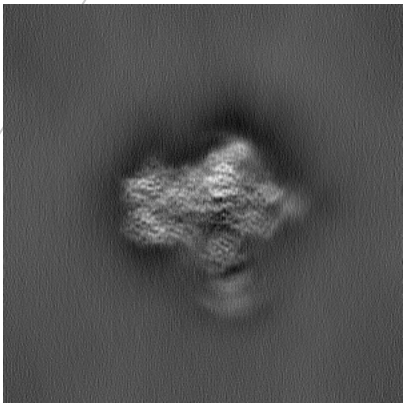


Z

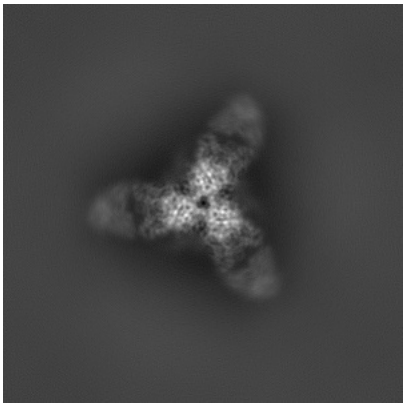
6.1.2 Raw map



X



Y

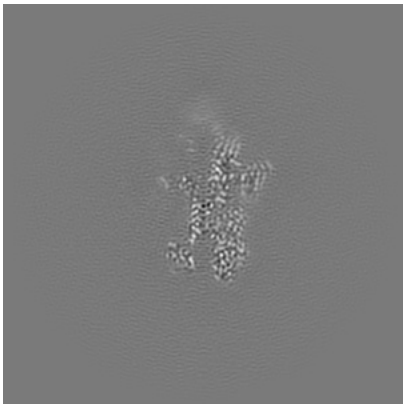


Z

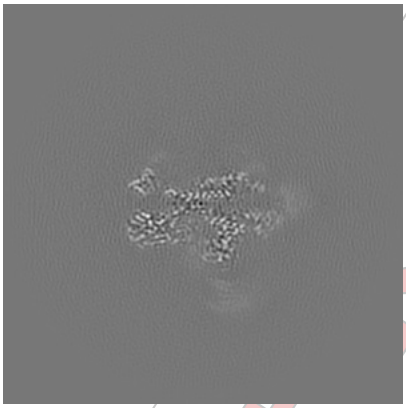
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

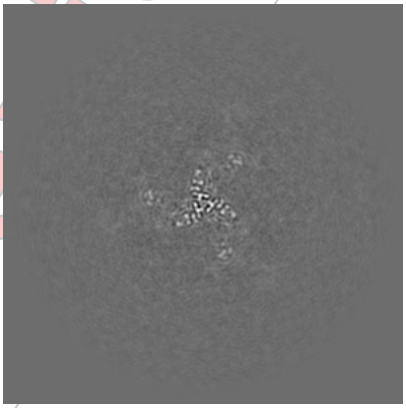
6.2.1 Primary map



X Index: 220

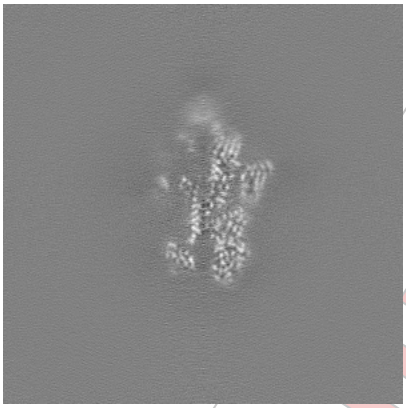


Y Index: 220

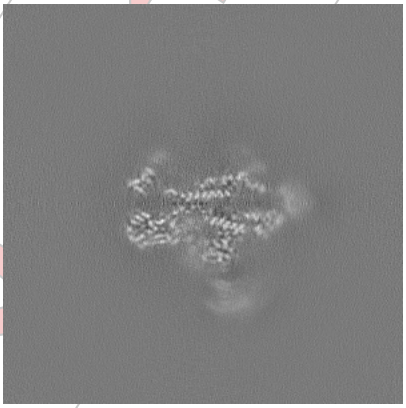


Z Index: 220

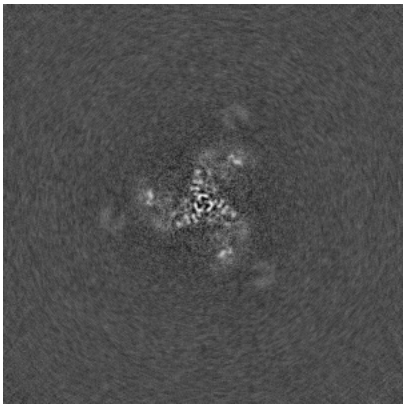
6.2.2 Raw map



X Index: 220



Y Index: 220

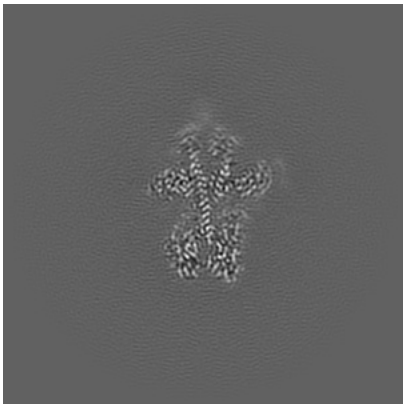


Z Index: 220

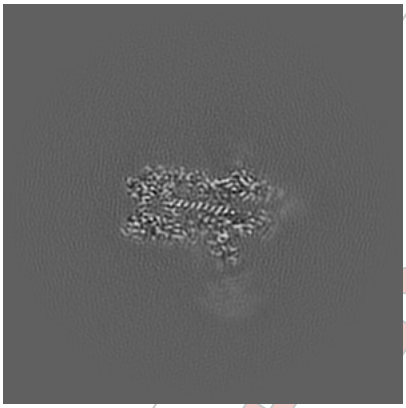
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

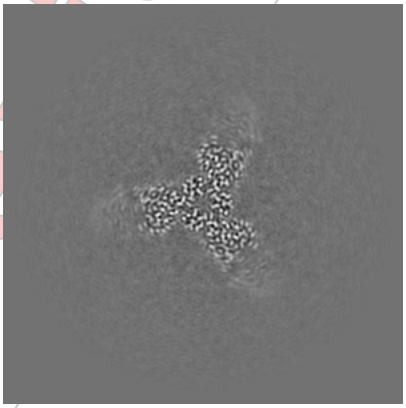
6.3.1 Primary map



X Index: 230

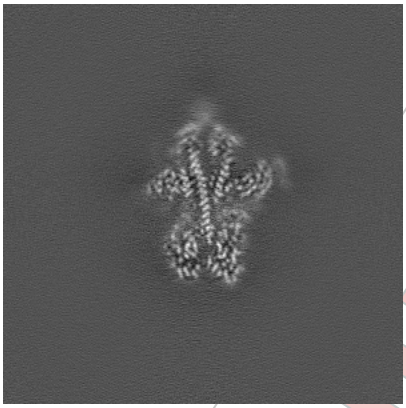


Y Index: 209

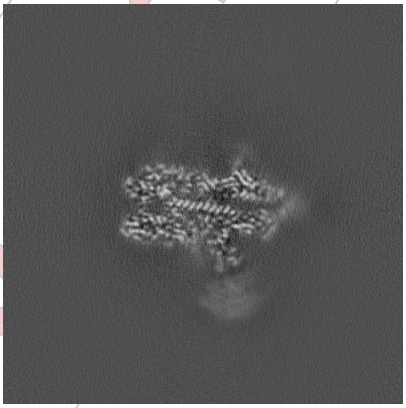


Z Index: 243

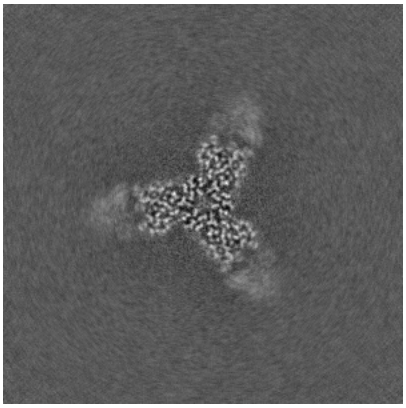
6.3.2 Raw map



X Index: 230



Y Index: 210

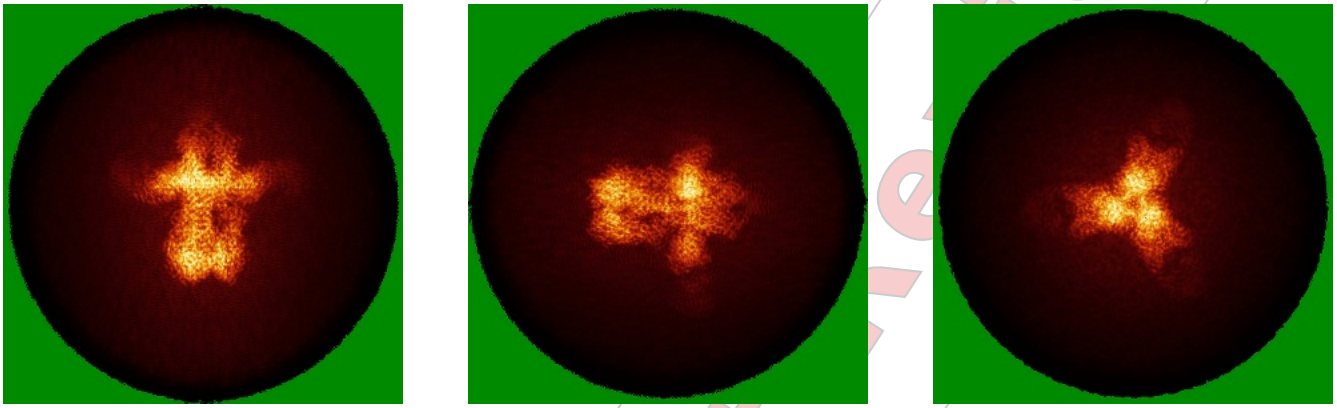


Z Index: 243

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

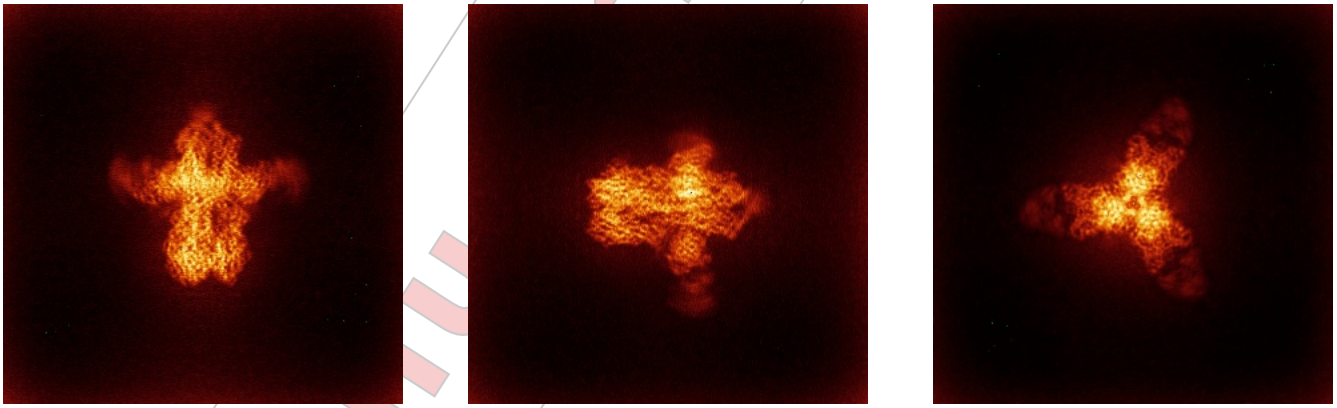
6.4 Orthogonal standard-deviation projections (False-color)

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

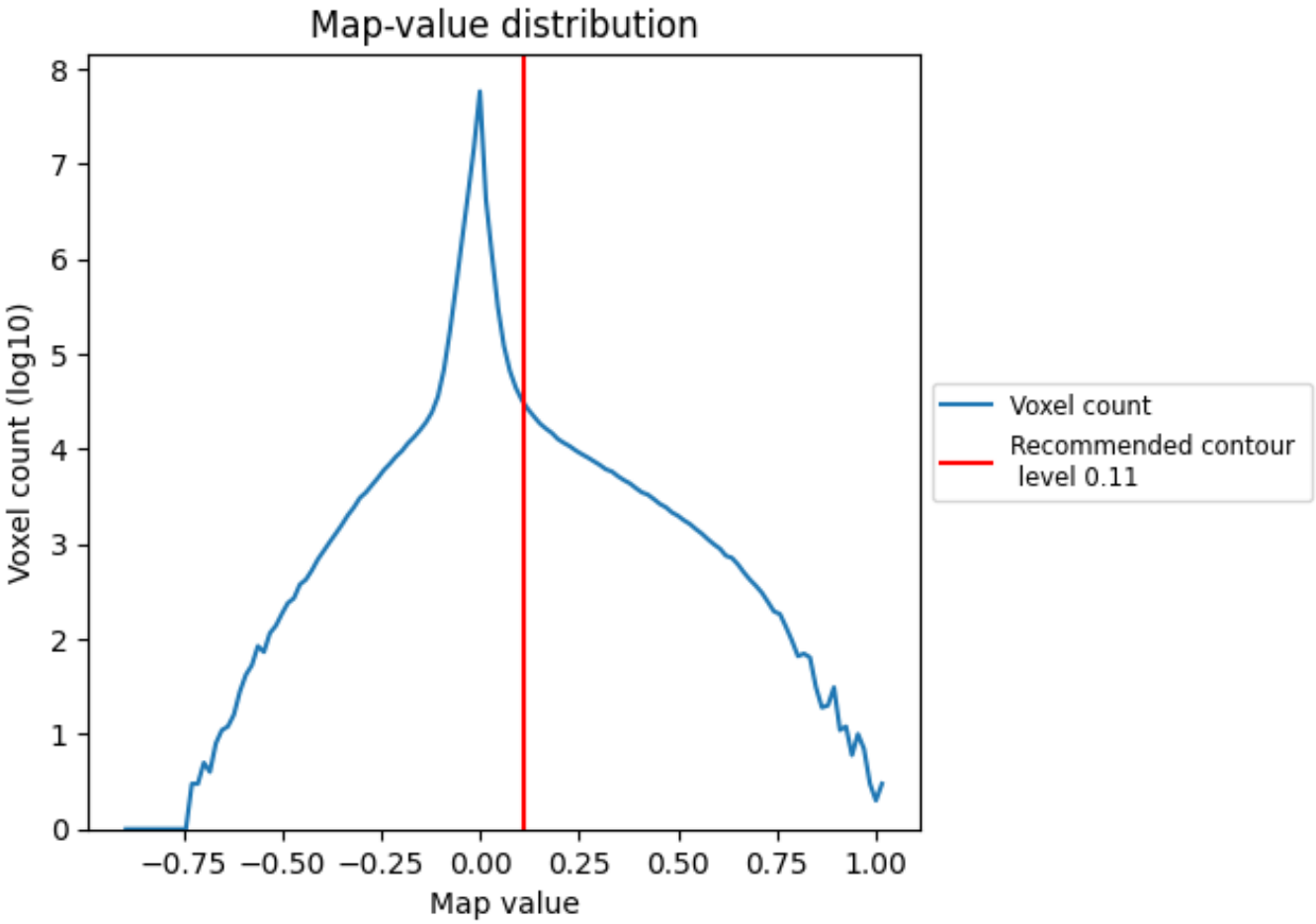
6.6 Mask visualisation (i)

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

7 Map analysis

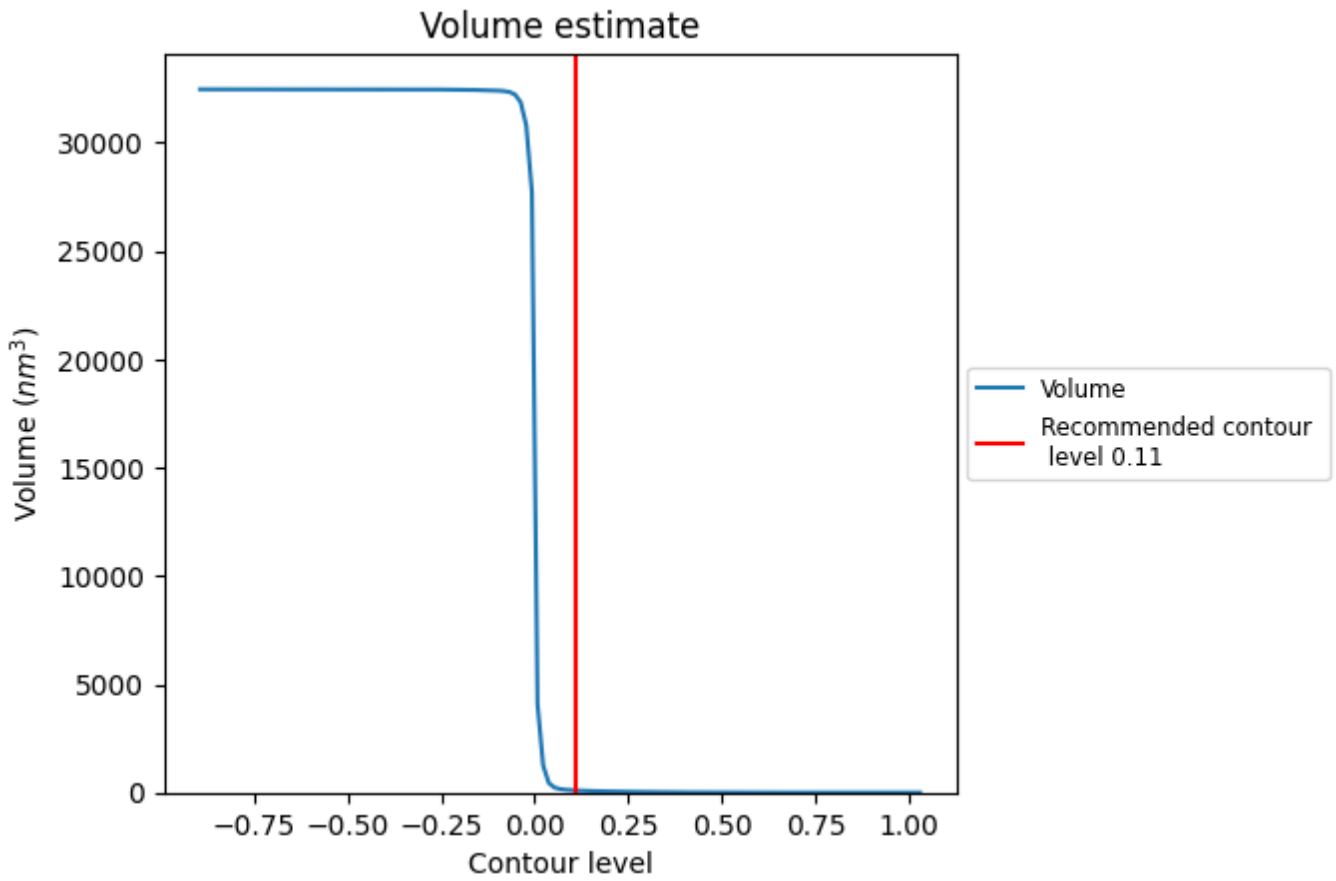
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

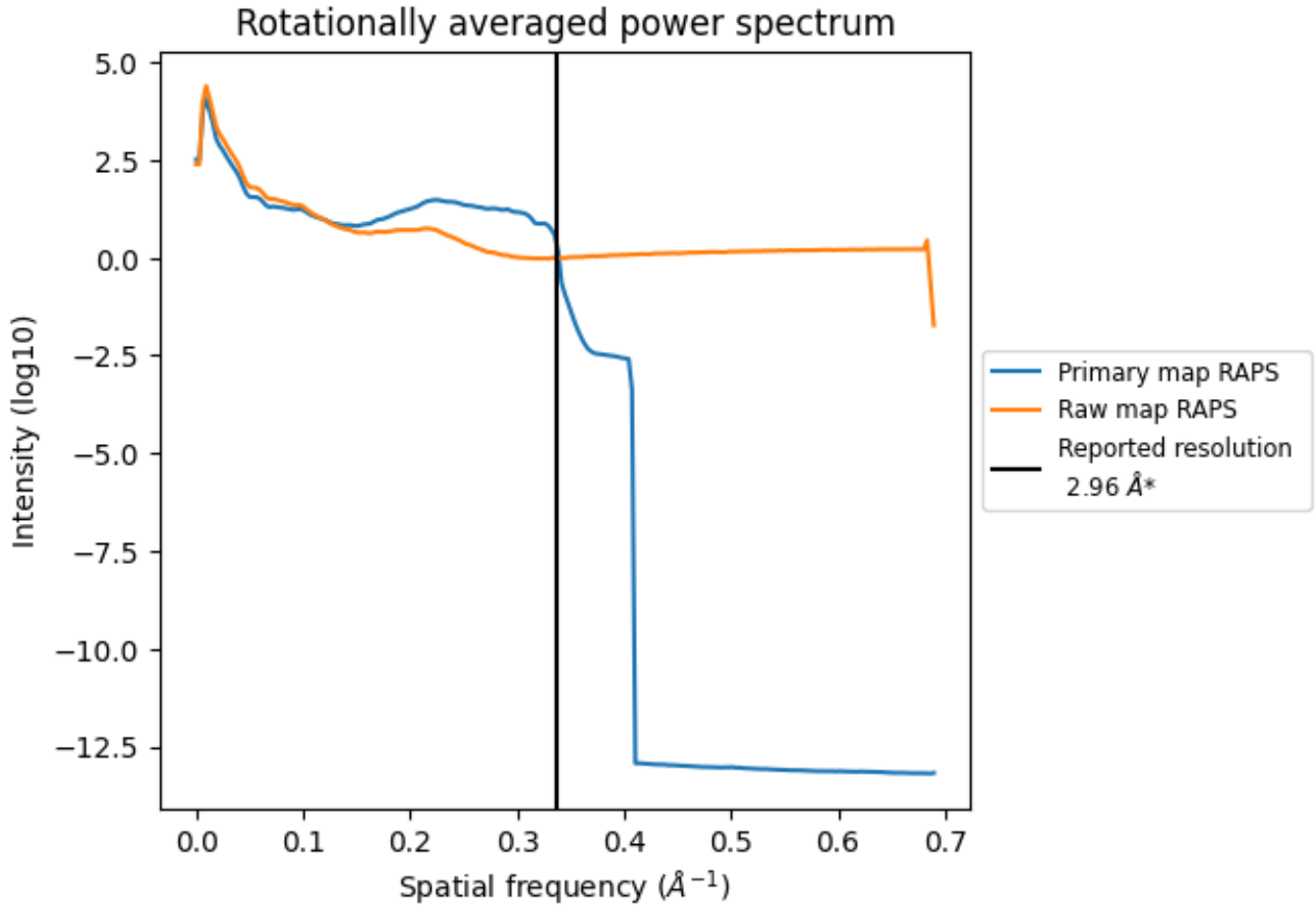
7.2 Volume estimate (i)



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 89 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)

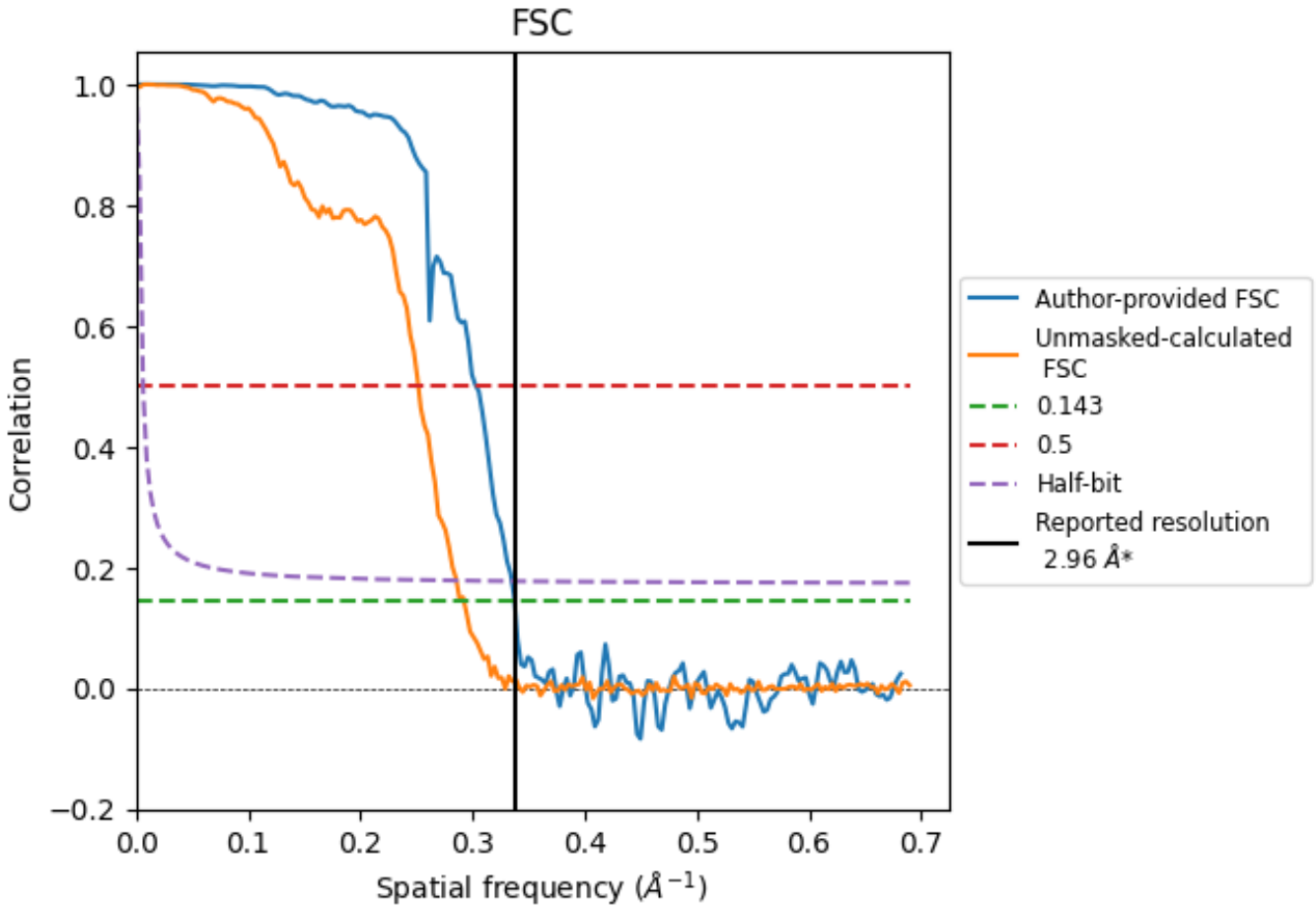


*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

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 0.338 Å^{-1}

8.2 Resolution estimates (i)

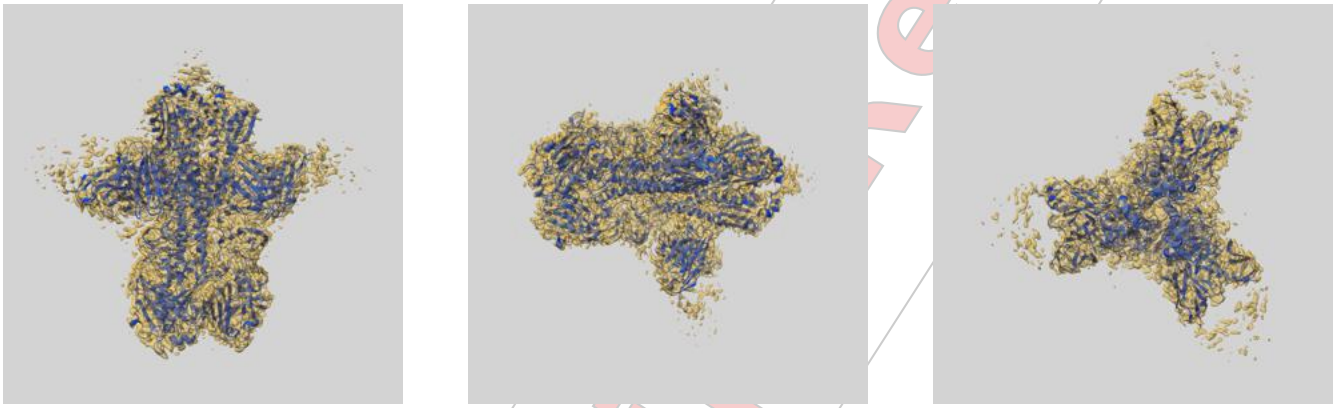
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.30	2.99
Unmasked-calculated*	3.42	3.97	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.96 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70234 and PDB model 9O8R. Per-residue inclusion information can be found in section 3 on page 12.

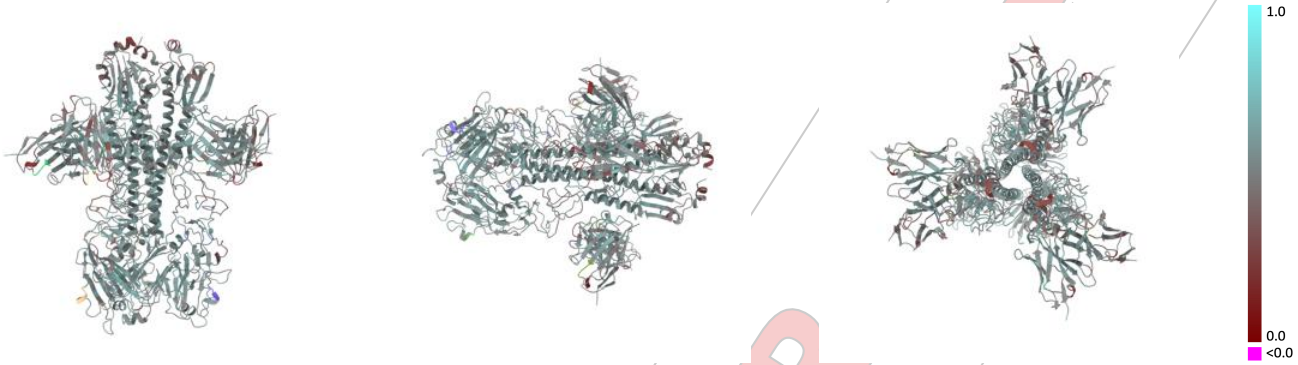
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

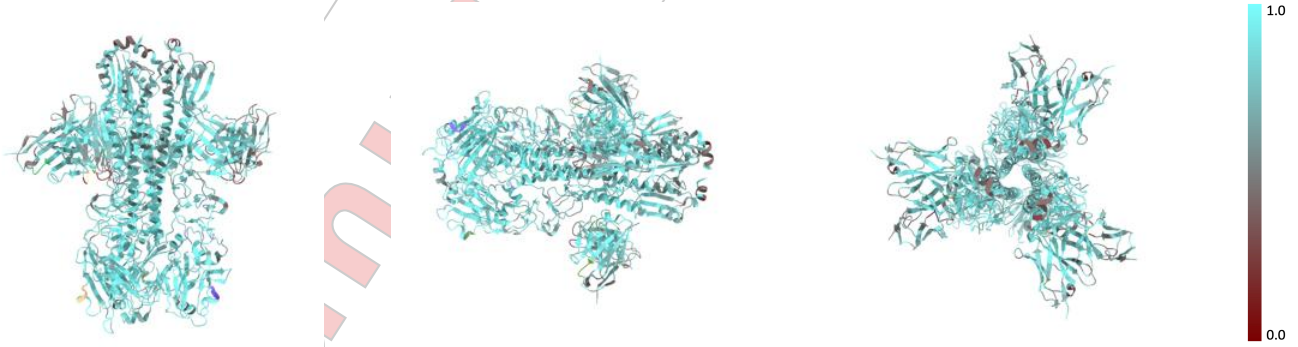
9.2 Q-score mapped to coordinate model



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.

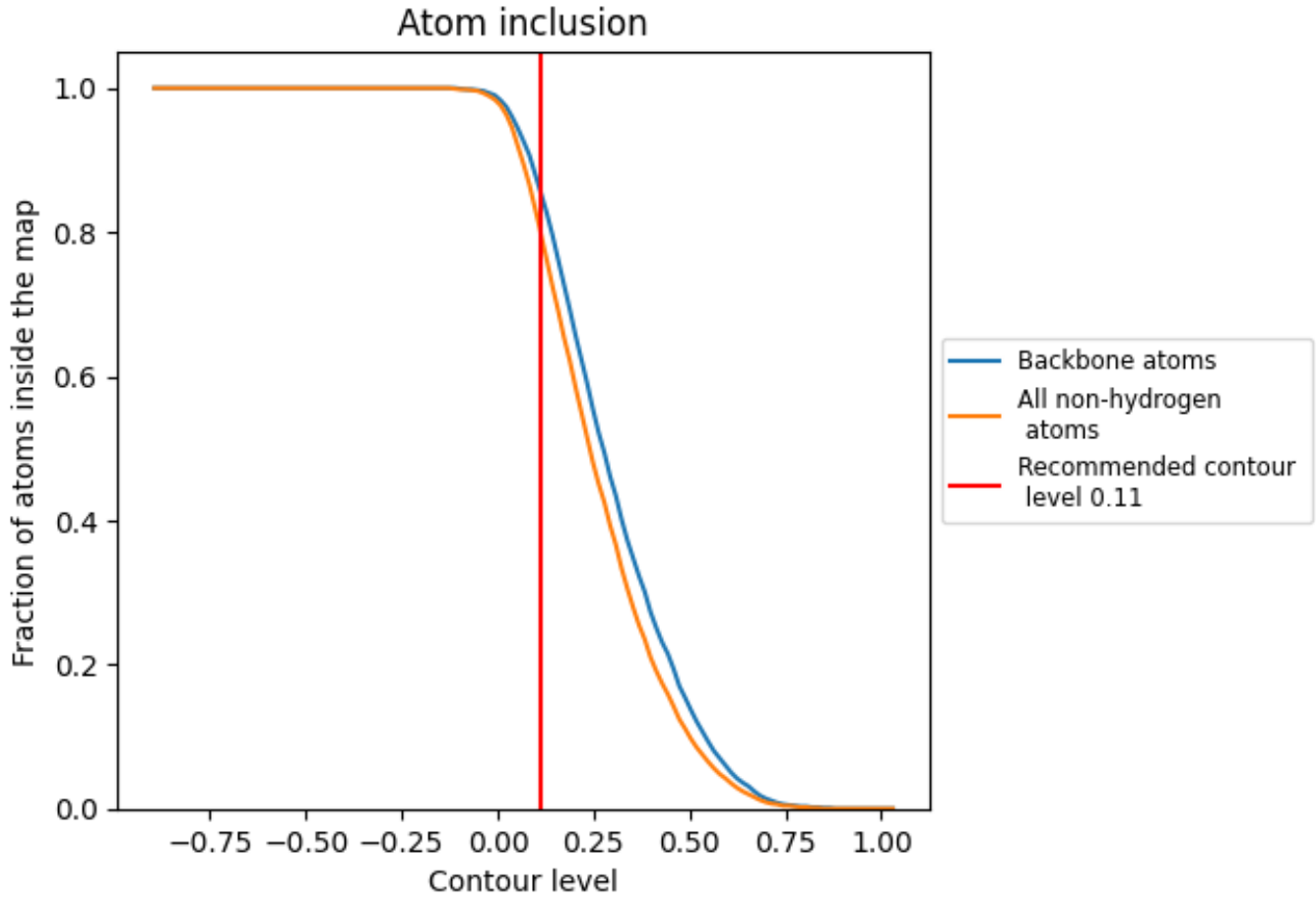
9.3 Atom inclusion mapped to coordinate model



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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.5280
A	0.8400	0.5400
B	0.7910	0.5210
C	0.8370	0.5410
D	0.8380	0.5400
E	0.7920	0.5210
F	0.7910	0.5200
G	0.8130	0.5350
H	0.8180	0.5330
I	0.8160	0.5340
J	0.7050	0.4920
K	0.7070	0.4900
L	0.7010	0.4850
M	0.7860	0.5200
N	0.7860	0.5180
O	0.7860	0.5200

Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 01:16 PM EDT

PDB ID	:	9O8S / pdb_00009o8s
EMDB ID	:	EMD-70235
Title	:	Cryo-EM structure of NI04359_d30_240 Fab in complex with influenza virus hemagglutinin from A/Hong Kong/485197/2014 (H3N2)
Deposited on	:	2025-04-16
Resolution	:	2.65 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 ①) were used in the production of this report:

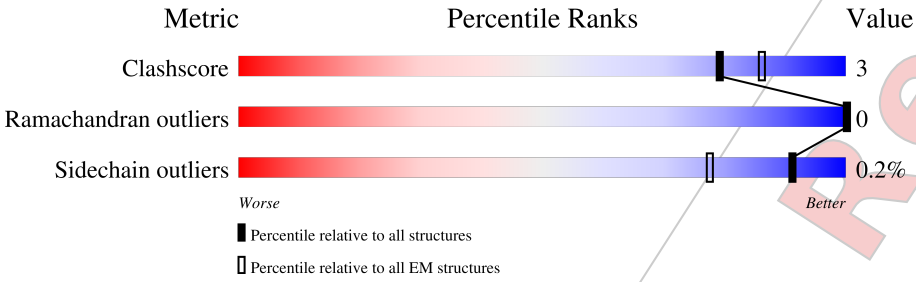
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.65 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	345	84% 7% • 8%
1	C	345	84% 7% • 8%
1	D	345	84% 7% • 8%
2	B	236	65% 8% 27%
2	E	236	65% 8% 27%
2	F	236	67% 5% 27%
3	G	130	18% 92% 7% •

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Mol	Chain	Length	Quality of chain
3	H	130	19% 92% 7%
3	I	130	18% 92% 7%
4	J	107	13% 92% 7%
4	K	107	13% 92% 7%
4	L	107	13% 93% 6%
5	M	2	50% 100%
5	O	2	50% 50%
5	R	2	50% 100%
5	T	2	50% 50%
5	W	2	50% 100%
5	Y	2	100%
6	N	3	100%
6	S	3	100%
6	X	3	100%
7	P	3	33% 67%
7	Q	3	33% 33% 33% 33%
7	U	3	33% 67%
7	V	3	33% 33% 67%
7	Z	3	33% 67%
7	a	3	33% 67% 33%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 17628 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	316	Total	C	N	O	S	0	0
			2471	1549	439	471	12		
1	C	316	Total	C	N	O	S	0	0
			2471	1549	439	471	12		
1	D	316	Total	C	N	O	S	0	0
			2471	1549	439	471	12		

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	172	Total	C	N	O	S	0	0
			1388	863	246	273	6		
2	E	172	Total	C	N	O	S	0	0
			1388	863	246	273	6		
2	F	172	Total	C	N	O	S	0	0
			1388	863	246	273	6		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLY	-	expression tag	UNP A0A0K0YAS1
B	178	TYR	-	expression tag	UNP A0A0K0YAS1
B	179	ILE	-	expression tag	UNP A0A0K0YAS1
B	180	PRO	-	expression tag	UNP A0A0K0YAS1
B	181	GLU	-	expression tag	UNP A0A0K0YAS1
B	182	ALA	-	expression tag	UNP A0A0K0YAS1
B	183	PRO	-	expression tag	UNP A0A0K0YAS1
B	184	ARG	-	expression tag	UNP A0A0K0YAS1
B	185	ASP	-	expression tag	UNP A0A0K0YAS1
B	186	GLY	-	expression tag	UNP A0A0K0YAS1
B	187	GLN	-	expression tag	UNP A0A0K0YAS1
B	188	ALA	-	expression tag	UNP A0A0K0YAS1
B	189	TYR	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	190	VAL	-	expression tag	UNP A0A0K0YAS1
B	191	ARG	-	expression tag	UNP A0A0K0YAS1
B	192	LYS	-	expression tag	UNP A0A0K0YAS1
B	193	ASP	-	expression tag	UNP A0A0K0YAS1
B	194	GLY	-	expression tag	UNP A0A0K0YAS1
B	195	GLU	-	expression tag	UNP A0A0K0YAS1
B	196	TRP	-	expression tag	UNP A0A0K0YAS1
B	197	VAL	-	expression tag	UNP A0A0K0YAS1
B	198	LEU	-	expression tag	UNP A0A0K0YAS1
B	199	LEU	-	expression tag	UNP A0A0K0YAS1
B	200	SER	-	expression tag	UNP A0A0K0YAS1
B	201	THR	-	expression tag	UNP A0A0K0YAS1
B	202	PHE	-	expression tag	UNP A0A0K0YAS1
B	203	LEU	-	expression tag	UNP A0A0K0YAS1
B	204	GLY	-	expression tag	UNP A0A0K0YAS1
B	205	SER	-	expression tag	UNP A0A0K0YAS1
B	206	GLU	-	expression tag	UNP A0A0K0YAS1
B	207	ASN	-	expression tag	UNP A0A0K0YAS1
B	208	LEU	-	expression tag	UNP A0A0K0YAS1
B	209	TYR	-	expression tag	UNP A0A0K0YAS1
B	210	PHE	-	expression tag	UNP A0A0K0YAS1
B	211	GLN	-	expression tag	UNP A0A0K0YAS1
B	212	GLY	-	expression tag	UNP A0A0K0YAS1
B	213	SER	-	expression tag	UNP A0A0K0YAS1
B	214	ALA	-	expression tag	UNP A0A0K0YAS1
B	215	TRP	-	expression tag	UNP A0A0K0YAS1
B	216	SER	-	expression tag	UNP A0A0K0YAS1
B	217	HIS	-	expression tag	UNP A0A0K0YAS1
B	218	PRO	-	expression tag	UNP A0A0K0YAS1
B	219	GLN	-	expression tag	UNP A0A0K0YAS1
B	220	PHE	-	expression tag	UNP A0A0K0YAS1
B	221	GLU	-	expression tag	UNP A0A0K0YAS1
B	222	LYS	-	expression tag	UNP A0A0K0YAS1
B	223	GLY	-	expression tag	UNP A0A0K0YAS1
B	224	GLY	-	expression tag	UNP A0A0K0YAS1
B	225	GLY	-	expression tag	UNP A0A0K0YAS1
B	226	SER	-	expression tag	UNP A0A0K0YAS1
B	227	GLY	-	expression tag	UNP A0A0K0YAS1
B	228	GLY	-	expression tag	UNP A0A0K0YAS1
B	229	GLY	-	expression tag	UNP A0A0K0YAS1
B	230	SER	-	expression tag	UNP A0A0K0YAS1
B	231	HIS	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	232	HIS	-	expression tag	UNP A0A0K0YAS1
B	233	HIS	-	expression tag	UNP A0A0K0YAS1
B	234	HIS	-	expression tag	UNP A0A0K0YAS1
B	235	HIS	-	expression tag	UNP A0A0K0YAS1
B	236	HIS	-	expression tag	UNP A0A0K0YAS1
E	177	GLY	-	expression tag	UNP A0A0K0YAS1
E	178	TYR	-	expression tag	UNP A0A0K0YAS1
E	179	ILE	-	expression tag	UNP A0A0K0YAS1
E	180	PRO	-	expression tag	UNP A0A0K0YAS1
E	181	GLU	-	expression tag	UNP A0A0K0YAS1
E	182	ALA	-	expression tag	UNP A0A0K0YAS1
E	183	PRO	-	expression tag	UNP A0A0K0YAS1
E	184	ARG	-	expression tag	UNP A0A0K0YAS1
E	185	ASP	-	expression tag	UNP A0A0K0YAS1
E	186	GLY	-	expression tag	UNP A0A0K0YAS1
E	187	GLN	-	expression tag	UNP A0A0K0YAS1
E	188	ALA	-	expression tag	UNP A0A0K0YAS1
E	189	TYR	-	expression tag	UNP A0A0K0YAS1
E	190	VAL	-	expression tag	UNP A0A0K0YAS1
E	191	ARG	-	expression tag	UNP A0A0K0YAS1
E	192	LYS	-	expression tag	UNP A0A0K0YAS1
E	193	ASP	-	expression tag	UNP A0A0K0YAS1
E	194	GLY	-	expression tag	UNP A0A0K0YAS1
E	195	GLU	-	expression tag	UNP A0A0K0YAS1
E	196	TRP	-	expression tag	UNP A0A0K0YAS1
E	197	VAL	-	expression tag	UNP A0A0K0YAS1
E	198	LEU	-	expression tag	UNP A0A0K0YAS1
E	199	LEU	-	expression tag	UNP A0A0K0YAS1
E	200	SER	-	expression tag	UNP A0A0K0YAS1
E	201	THR	-	expression tag	UNP A0A0K0YAS1
E	202	PHE	-	expression tag	UNP A0A0K0YAS1
E	203	LEU	-	expression tag	UNP A0A0K0YAS1
E	204	GLY	-	expression tag	UNP A0A0K0YAS1
E	205	SER	-	expression tag	UNP A0A0K0YAS1
E	206	GLU	-	expression tag	UNP A0A0K0YAS1
E	207	ASN	-	expression tag	UNP A0A0K0YAS1
E	208	LEU	-	expression tag	UNP A0A0K0YAS1
E	209	TYR	-	expression tag	UNP A0A0K0YAS1
E	210	PHE	-	expression tag	UNP A0A0K0YAS1
E	211	GLN	-	expression tag	UNP A0A0K0YAS1
E	212	GLY	-	expression tag	UNP A0A0K0YAS1
E	213	SER	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	214	ALA	-	expression tag	UNP A0A0K0YAS1
E	215	TRP	-	expression tag	UNP A0A0K0YAS1
E	216	SER	-	expression tag	UNP A0A0K0YAS1
E	217	HIS	-	expression tag	UNP A0A0K0YAS1
E	218	PRO	-	expression tag	UNP A0A0K0YAS1
E	219	GLN	-	expression tag	UNP A0A0K0YAS1
E	220	PHE	-	expression tag	UNP A0A0K0YAS1
E	221	GLU	-	expression tag	UNP A0A0K0YAS1
E	222	LYS	-	expression tag	UNP A0A0K0YAS1
E	223	GLY	-	expression tag	UNP A0A0K0YAS1
E	224	GLY	-	expression tag	UNP A0A0K0YAS1
E	225	GLY	-	expression tag	UNP A0A0K0YAS1
E	226	SER	-	expression tag	UNP A0A0K0YAS1
E	227	GLY	-	expression tag	UNP A0A0K0YAS1
E	228	GLY	-	expression tag	UNP A0A0K0YAS1
E	229	GLY	-	expression tag	UNP A0A0K0YAS1
E	230	SER	-	expression tag	UNP A0A0K0YAS1
E	231	HIS	-	expression tag	UNP A0A0K0YAS1
E	232	HIS	-	expression tag	UNP A0A0K0YAS1
E	233	HIS	-	expression tag	UNP A0A0K0YAS1
E	234	HIS	-	expression tag	UNP A0A0K0YAS1
E	235	HIS	-	expression tag	UNP A0A0K0YAS1
E	236	HIS	-	expression tag	UNP A0A0K0YAS1
F	177	GLY	-	expression tag	UNP A0A0K0YAS1
F	178	TYR	-	expression tag	UNP A0A0K0YAS1
F	179	ILE	-	expression tag	UNP A0A0K0YAS1
F	180	PRO	-	expression tag	UNP A0A0K0YAS1
F	181	GLU	-	expression tag	UNP A0A0K0YAS1
F	182	ALA	-	expression tag	UNP A0A0K0YAS1
F	183	PRO	-	expression tag	UNP A0A0K0YAS1
F	184	ARG	-	expression tag	UNP A0A0K0YAS1
F	185	ASP	-	expression tag	UNP A0A0K0YAS1
F	186	GLY	-	expression tag	UNP A0A0K0YAS1
F	187	GLN	-	expression tag	UNP A0A0K0YAS1
F	188	ALA	-	expression tag	UNP A0A0K0YAS1
F	189	TYR	-	expression tag	UNP A0A0K0YAS1
F	190	VAL	-	expression tag	UNP A0A0K0YAS1
F	191	ARG	-	expression tag	UNP A0A0K0YAS1
F	192	LYS	-	expression tag	UNP A0A0K0YAS1
F	193	ASP	-	expression tag	UNP A0A0K0YAS1
F	194	GLY	-	expression tag	UNP A0A0K0YAS1
F	195	GLU	-	expression tag	UNP A0A0K0YAS1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	196	TRP	-	expression tag	UNP A0A0K0YAS1
F	197	VAL	-	expression tag	UNP A0A0K0YAS1
F	198	LEU	-	expression tag	UNP A0A0K0YAS1
F	199	LEU	-	expression tag	UNP A0A0K0YAS1
F	200	SER	-	expression tag	UNP A0A0K0YAS1
F	201	THR	-	expression tag	UNP A0A0K0YAS1
F	202	PHE	-	expression tag	UNP A0A0K0YAS1
F	203	LEU	-	expression tag	UNP A0A0K0YAS1
F	204	GLY	-	expression tag	UNP A0A0K0YAS1
F	205	SER	-	expression tag	UNP A0A0K0YAS1
F	206	GLU	-	expression tag	UNP A0A0K0YAS1
F	207	ASN	-	expression tag	UNP A0A0K0YAS1
F	208	LEU	-	expression tag	UNP A0A0K0YAS1
F	209	TYR	-	expression tag	UNP A0A0K0YAS1
F	210	PHE	-	expression tag	UNP A0A0K0YAS1
F	211	GLN	-	expression tag	UNP A0A0K0YAS1
F	212	GLY	-	expression tag	UNP A0A0K0YAS1
F	213	SER	-	expression tag	UNP A0A0K0YAS1
F	214	ALA	-	expression tag	UNP A0A0K0YAS1
F	215	TRP	-	expression tag	UNP A0A0K0YAS1
F	216	SER	-	expression tag	UNP A0A0K0YAS1
F	217	HIS	-	expression tag	UNP A0A0K0YAS1
F	218	PRO	-	expression tag	UNP A0A0K0YAS1
F	219	GLN	-	expression tag	UNP A0A0K0YAS1
F	220	PHE	-	expression tag	UNP A0A0K0YAS1
F	221	GLU	-	expression tag	UNP A0A0K0YAS1
F	222	LYS	-	expression tag	UNP A0A0K0YAS1
F	223	GLY	-	expression tag	UNP A0A0K0YAS1
F	224	GLY	-	expression tag	UNP A0A0K0YAS1
F	225	GLY	-	expression tag	UNP A0A0K0YAS1
F	226	SER	-	expression tag	UNP A0A0K0YAS1
F	227	GLY	-	expression tag	UNP A0A0K0YAS1
F	228	GLY	-	expression tag	UNP A0A0K0YAS1
F	229	GLY	-	expression tag	UNP A0A0K0YAS1
F	230	SER	-	expression tag	UNP A0A0K0YAS1
F	231	HIS	-	expression tag	UNP A0A0K0YAS1
F	232	HIS	-	expression tag	UNP A0A0K0YAS1
F	233	HIS	-	expression tag	UNP A0A0K0YAS1
F	234	HIS	-	expression tag	UNP A0A0K0YAS1
F	235	HIS	-	expression tag	UNP A0A0K0YAS1
F	236	HIS	-	expression tag	UNP A0A0K0YAS1

- Molecule 3 is a protein called NI04359_d30_240 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	128	Total	C	N	O	S	0	0
			971	608	167	189	7		
3	G	128	Total	C	N	O	S	0	0
			971	608	167	189	7		
3	I	128	Total	C	N	O	S	0	0
			971	608	167	189	7		

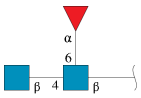
- Molecule 4 is a protein called NI04359_d30_240 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	105	Total	C	N	O	S	0	0
			790	492	129	166	3		
4	J	105	Total	C	N	O	S	0	0
			790	492	129	166	3		
4	K	105	Total	C	N	O	S	0	0
			790	492	129	166	3		

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

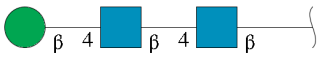
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		

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



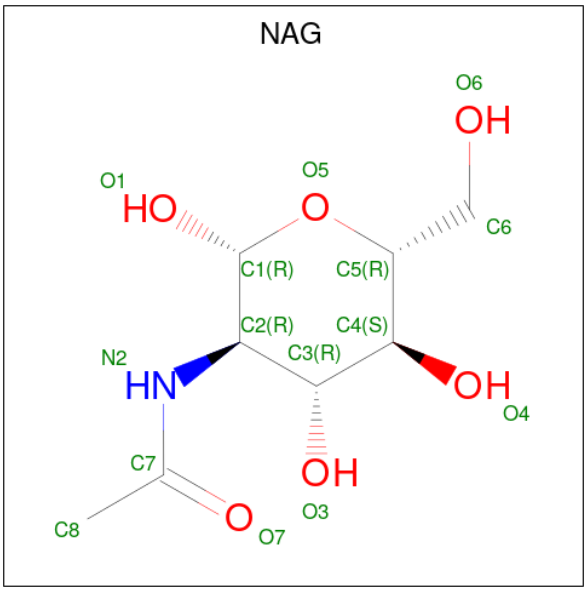
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	3	Total	C	N	O	0	0
			38	22	2	14		
6	S	3	Total	C	N	O	0	0
			38	22	2	14		
6	X	3	Total	C	N	O	0	0
			38	22	2	14		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	3	Total	C	N	O	0	0
			39	22	2	15		
7	Q	3	Total	C	N	O	0	0
			39	22	2	15		
7	U	3	Total	C	N	O	0	0
			39	22	2	15		
7	V	3	Total	C	N	O	0	0
			39	22	2	15		
7	Z	3	Total	C	N	O	0	0
			39	22	2	15		
7	a	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

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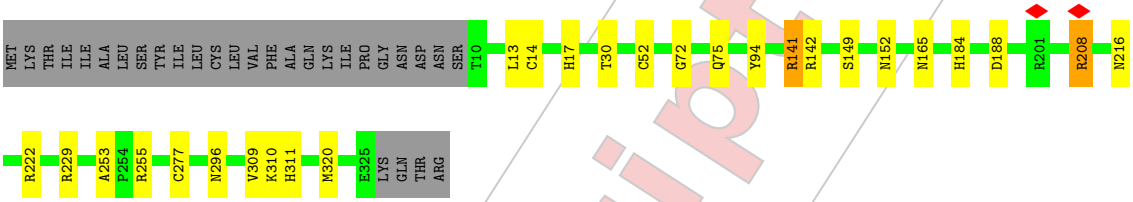
Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

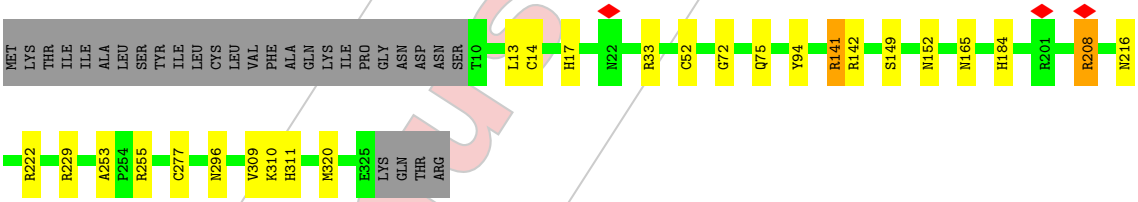
- Molecule 1: Hemagglutinin HA1

Chain A:



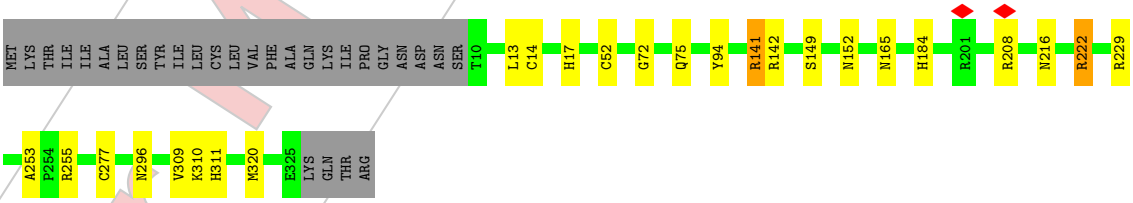
- Molecule 1: Hemagglutinin HA1

Chain C:



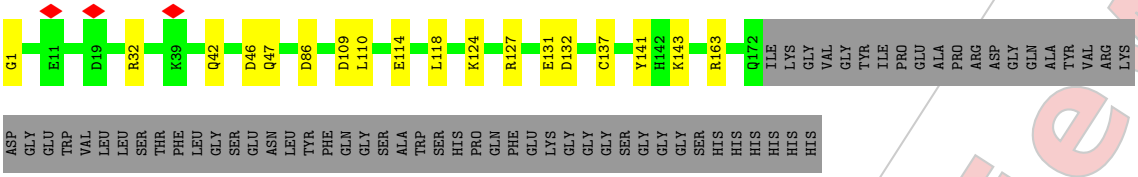
- Molecule 1: Hemagglutinin HA1

Chain D:



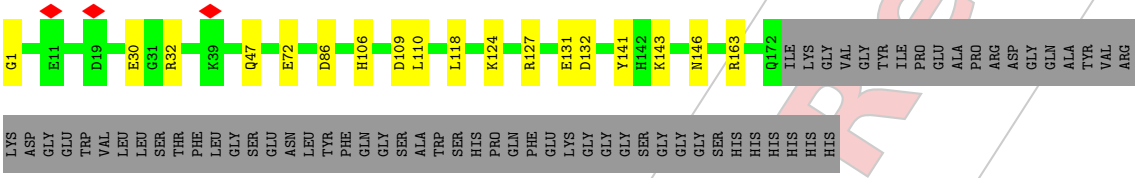
- Molecule 2: Hemagglutinin HA2

Chain B:



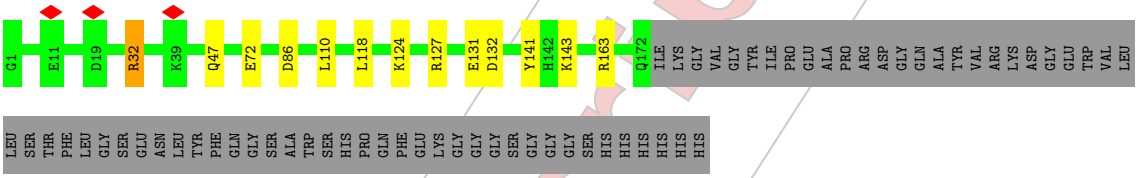
• Molecule 2: Hemagglutinin HA2

Chain E:



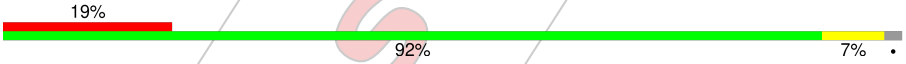
• Molecule 2: Hemagglutinin HA2

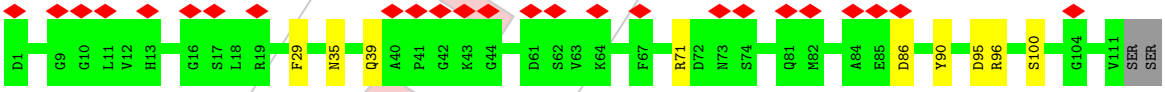
Chain F:



• Molecule 3: NI04359_d30_240 Fab heavy chain

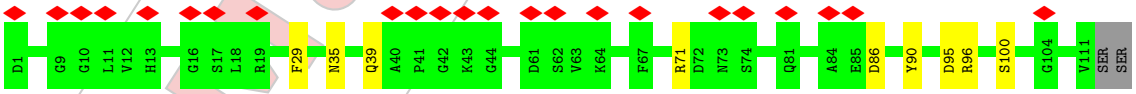
Chain H:





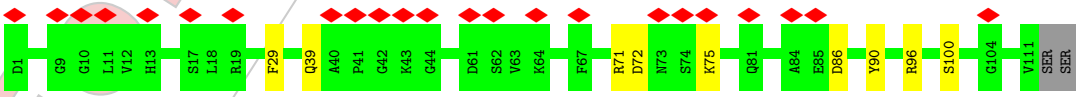
• Molecule 3: NI04359_d30_240 Fab heavy chain

Chain G:



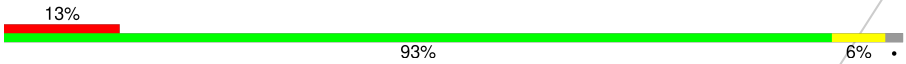
• Molecule 3: NI04359_d30_240 Fab heavy chain

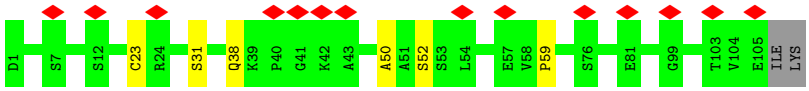
Chain I:



• Molecule 4: NI04359_d30_240 Fab light chain

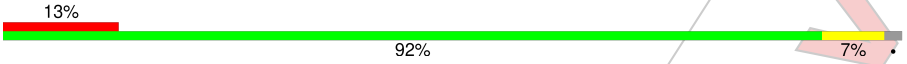
Chain L:

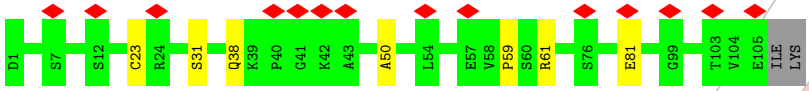




• Molecule 4: NI04359_d30_240 Fab light chain

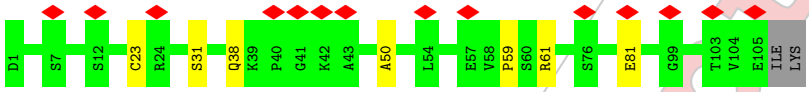
Chain J:





• Molecule 4: NI04359_d30_240 Fab light chain

Chain K:



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

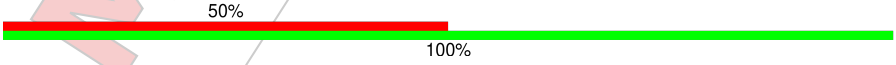
Chain M:

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

Chain O:

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

Chain R:



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

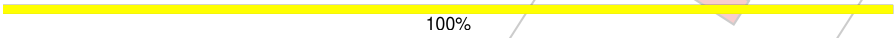
Chain T:

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

Chain W:

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

Chain Y:

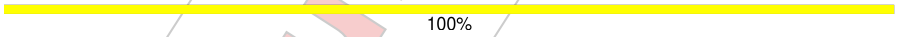


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

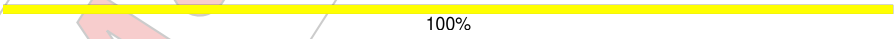
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



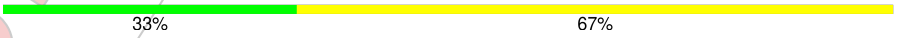
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



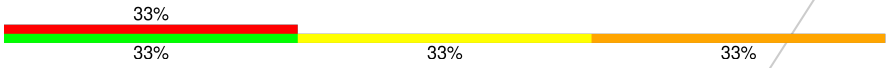
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



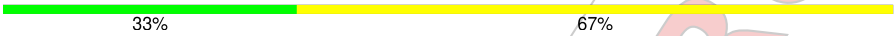
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain U:



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

Chain V:

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

Chain Z:

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

Chain a:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	196828	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45.09	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	190000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.373	Depositor
Minimum map value	-0.210	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	315.91998, 315.91998, 315.91998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71799994, 0.71799994, 0.71799994	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, FUC

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	0.40	3/2528 (0.1%)	0.70	4/3439 (0.1%)
1	C	0.40	3/2528 (0.1%)	0.70	3/3439 (0.1%)
1	D	0.40	3/2528 (0.1%)	0.70	3/3439 (0.1%)
2	B	0.39	0/1412	0.73	3/1895 (0.2%)
2	E	0.39	0/1412	0.71	1/1895 (0.1%)
2	F	0.36	0/1412	0.70	3/1895 (0.2%)
3	G	0.34	0/993	0.65	0/1343
3	H	0.34	0/993	0.68	0/1343
3	I	0.39	0/993	0.68	0/1343
4	J	0.32	0/807	0.70	2/1097 (0.2%)
4	K	0.33	0/807	0.69	2/1097 (0.2%)
4	L	0.33	0/807	0.71	2/1097 (0.2%)
All	All	0.38	9/17220 (0.1%)	0.70	23/23322 (0.1%)

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	5
1	C	0	4
1	D	0	5
2	B	0	1
2	E	0	1
2	F	0	1
All	All	0	17

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	277	CYS	CB-SG	-7.85	1.69	1.82
1	D	277	CYS	CB-SG	-7.82	1.69	1.82
1	C	52	CYS	CB-SG	7.81	1.95	1.82
1	A	277	CYS	CB-SG	-7.80	1.69	1.82
1	A	52	CYS	CB-SG	7.77	1.95	1.82
1	D	52	CYS	CB-SG	7.75	1.95	1.82
1	A	14	CYS	CB-SG	-5.61	1.72	1.81
1	C	14	CYS	CB-SG	-5.34	1.73	1.81
1	D	14	CYS	CB-SG	-5.07	1.73	1.81

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	277	CYS	CA-CB-SG	10.47	132.85	114.00
1	D	277	CYS	CA-CB-SG	10.45	132.82	114.00
1	A	277	CYS	CA-CB-SG	10.41	132.74	114.00
1	D	13	LEU	CA-CB-CG	6.84	131.04	115.30
1	C	13	LEU	CA-CB-CG	6.83	131.02	115.30
1	A	188	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	13	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	277	CYS	CB-CA-C	-5.99	98.42	110.40
1	D	277	CYS	CB-CA-C	-5.97	98.46	110.40
1	C	277	CYS	CB-CA-C	-5.96	98.49	110.40
2	B	110	LEU	CA-CB-CG	5.86	128.78	115.30
4	L	23	CYS	CA-CB-SG	5.72	124.31	114.00
4	J	23	CYS	CA-CB-SG	5.71	124.28	114.00
4	K	23	CYS	CA-CB-SG	5.43	123.78	114.00
2	E	118	LEU	CA-CB-CG	5.31	127.51	115.30
4	L	59	PRO	CA-N-CD	-5.21	104.20	111.50
4	K	59	PRO	CA-N-CD	-5.21	104.21	111.50
4	J	59	PRO	CA-N-CD	-5.19	104.24	111.50
2	B	137	CYS	CA-CB-SG	5.18	123.32	114.00
2	F	110	LEU	CA-CB-CG	5.17	127.20	115.30
2	F	118	LEU	CA-CB-CG	5.16	127.18	115.30
2	F	32	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	118	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	229	ARG	Sidechain
2	B	32	ARG	Sidechain
1	C	141	ARG	Sidechain
1	C	142	ARG	Sidechain
1	C	208	ARG	Sidechain
1	C	229	ARG	Sidechain
1	D	141	ARG	Sidechain
1	D	142	ARG	Sidechain
1	D	208	ARG	Sidechain
1	D	222	ARG	Sidechain
1	D	229	ARG	Sidechain
2	E	32	ARG	Sidechain
2	F	32	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	2471	0	2416	12	0
1	C	2471	0	2417	14	0
1	D	2471	0	2416	14	0
2	B	1388	0	1318	10	0
2	E	1388	0	1318	12	0
2	F	1388	0	1318	9	0
3	G	971	0	919	6	0
3	H	971	0	919	6	0
3	I	971	0	919	6	0
4	J	790	0	756	4	0
4	K	790	0	756	4	0
4	L	790	0	756	4	0
5	M	28	0	25	0	0
5	O	28	0	25	2	0
5	R	28	0	25	0	0
5	T	28	0	25	2	0
5	W	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	28	0	25	2	0
6	N	38	0	34	0	0
6	S	38	0	34	0	0
6	X	38	0	34	0	0
7	P	39	0	34	0	0
7	Q	39	0	32	3	0
7	U	39	0	34	0	0
7	V	39	0	32	5	0
7	Z	39	0	34	0	0
7	a	39	0	32	0	0
8	A	70	0	65	0	0
8	B	14	0	13	0	0
8	C	70	0	65	0	0
8	D	70	0	65	0	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
All	All	17628	0	16912	87	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 (87) 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:208:ARG:NH2	2:F:72:GLU:OE2	2.23	0.72
1:A:208:ARG:NH2	2:E:72:GLU:OE2	2.23	0.71
3:I:72:ASP:OD2	3:I:75:LYS:NZ	2.18	0.71
3:I:29:PHE:O	3:I:71:ARG:NH2	2.24	0.70
3:H:29:PHE:O	3:H:71:ARG:NH2	2.25	0.69
3:G:29:PHE:O	3:G:71:ARG:NH2	2.25	0.69
5:O:1:NAG:O3	5:O:2:NAG:O5	2.10	0.67
3:H:86:ASP:OD1	3:H:90:TYR:OH	2.13	0.67
5:T:1:NAG:O3	5:T:2:NAG:O5	2.11	0.65
5:O:1:NAG:O3	5:O:1:NAG:O7	2.16	0.64
5:T:1:NAG:O3	5:T:1:NAG:O7	2.16	0.64
5:Y:1:NAG:O3	5:Y:1:NAG:O7	2.16	0.64
5:Y:1:NAG:O3	5:Y:2:NAG:O5	2.11	0.63
1:C:72:GLY:O	1:C:141:ARG:NH2	2.33	0.61
1:D:72:GLY:O	1:D:141:ARG:NH2	2.34	0.61
3:H:35:ASN:ND2	3:H:95:ASP:OD1	2.34	0.60
3:G:86:ASP:OD1	3:G:90:TYR:OH	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:GLN:NE2	2:B:46:ASP:OD1	2.35	0.60
2:B:1:GLY:N	2:B:109:ASP:OD1	2.35	0.58
1:C:310:LYS:NZ	2:E:86:ASP:OD1	2.36	0.58
1:A:149:SER:O	1:A:255:ARG:NE	2.37	0.58
1:D:149:SER:O	1:D:255:ARG:NE	2.37	0.57
1:A:310:LYS:NZ	2:B:86:ASP:OD1	2.37	0.57
7:V:1:NAG:O7	7:V:1:NAG:O3	2.21	0.56
3:G:35:ASN:ND2	3:G:95:ASP:OD1	2.39	0.56
1:A:17:HIS:ND1	1:A:320:MET:SD	2.79	0.56
1:D:17:HIS:ND1	1:D:320:MET:SD	2.78	0.56
1:C:17:HIS:ND1	1:C:320:MET:SD	2.79	0.55
2:E:30:GLU:OE1	2:E:146:ASN:ND2	2.40	0.54
4:K:31:SER:OG	4:K:50:ALA:O	2.25	0.54
1:D:222:ARG:HD2	7:V:2:NAG:H82	1.90	0.54
2:B:163:ARG:NH2	2:E:131:GLU:OE2	2.41	0.54
4:L:31:SER:OG	4:L:50:ALA:O	2.26	0.54
7:Q:1:NAG:O7	7:Q:1:NAG:O3	2.21	0.54
1:C:149:SER:O	1:C:255:ARG:NE	2.37	0.54
3:H:39:GLN:OE1	4:L:38:GLN:NE2	2.42	0.53
1:D:310:LYS:NZ	2:F:86:ASP:OD1	2.41	0.53
1:A:30:THR:HG21	2:F:47:GLN:HE21	1.72	0.53
2:B:127:ARG:NH2	2:E:141:TYR:OH	2.41	0.53
2:B:131:GLU:OE2	2:F:163:ARG:NH2	2.42	0.53
1:D:222:ARG:HG3	7:V:2:NAG:H82	1.91	0.53
3:G:96:ARG:NH2	3:G:100:SER:O	2.42	0.53
3:H:96:ARG:NH2	3:H:100:SER:O	2.42	0.53
2:E:127:ARG:NH2	2:F:141:TYR:OH	2.42	0.53
2:E:163:ARG:NH2	2:F:131:GLU:OE2	2.42	0.52
3:I:39:GLN:OE1	4:K:38:GLN:NE2	2.42	0.52
3:G:39:GLN:OE1	4:J:38:GLN:NE2	2.42	0.52
2:B:141:TYR:OH	2:F:127:ARG:NH2	2.43	0.52
4:J:31:SER:OG	4:J:50:ALA:O	2.26	0.51
2:E:47:GLN:HE21	2:E:110:LEU:HD11	1.75	0.51
2:E:1:GLY:N	2:E:109:ASP:OD1	2.36	0.50
2:B:132:ASP:OD2	2:F:124:LYS:NZ	2.42	0.50
1:C:296:ASN:ND2	1:C:311:HIS:O	2.42	0.50
1:A:296:ASN:ND2	1:A:309:VAL:O	2.45	0.49
3:I:86:ASP:OD1	3:I:90:TYR:OH	2.23	0.49
2:B:124:LYS:NZ	2:E:132:ASP:OD2	2.42	0.48
1:D:296:ASN:ND2	1:D:311:HIS:O	2.40	0.48
1:A:165:ASN:N	1:A:165:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ASN:ND2	1:D:309:VAL:O	2.47	0.48
1:A:296:ASN:ND2	1:A:311:HIS:O	2.39	0.47
1:A:75:GLN:NE2	1:A:94:TYR:O	2.46	0.47
1:C:296:ASN:ND2	1:C:309:VAL:O	2.48	0.46
2:E:124:LYS:NZ	2:F:132:ASP:OD2	2.39	0.46
1:A:72:GLY:O	1:A:141:ARG:NH2	2.48	0.46
1:D:222:ARG:CG	7:V:2:NAG:H82	2.46	0.46
1:D:165:ASN:N	1:D:165:ASN:OD1	2.49	0.46
1:D:152:ASN:O	1:D:253:ALA:N	2.50	0.45
3:I:96:ARG:NH2	3:I:100:SER:O	2.49	0.45
1:C:222:ARG:HD2	7:Q:2:NAG:H82	1.99	0.44
1:C:184:HIS:HD1	1:C:216:ASN:H	1.65	0.44
1:D:184:HIS:HD1	1:D:216:ASN:H	1.65	0.43
1:C:152:ASN:O	1:C:253:ALA:N	2.49	0.43
1:A:184:HIS:HD1	1:A:216:ASN:H	1.66	0.42
2:B:47:GLN:NE2	2:B:114:GLU:OE2	2.53	0.42
4:K:61:ARG:NH2	4:K:81:GLU:OE2	2.50	0.42
1:D:222:ARG:CD	7:V:2:NAG:H82	2.50	0.41
3:G:39:GLN:NE2	4:J:38:GLN:OE1	2.53	0.41
3:I:39:GLN:NE2	4:K:38:GLN:OE1	2.54	0.41
3:H:39:GLN:NE2	4:L:38:GLN:OE1	2.54	0.41
1:C:75:GLN:NE2	1:C:94:TYR:O	2.51	0.41
1:C:222:ARG:NE	7:Q:2:NAG:O3	2.38	0.41
1:C:165:ASN:N	1:C:165:ASN:OD1	2.53	0.41
2:E:106:HIS:O	2:E:110:LEU:HB2	2.21	0.41
4:J:61:ARG:NH2	4:J:81:GLU:OE2	2.52	0.41
1:D:75:GLN:NE2	1:D:94:TYR:O	2.51	0.41
4:L:52:SER:O	1:C:33:ARG:NH1	2.55	0.40
1:A:152:ASN:O	1:A:253:ALA:N	2.50	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	314/345 (91%)	310 (99%)	4 (1%)	0	100	100
1	C	314/345 (91%)	310 (99%)	4 (1%)	0	100	100
1	D	314/345 (91%)	310 (99%)	4 (1%)	0	100	100
2	B	170/236 (72%)	166 (98%)	4 (2%)	0	100	100
2	E	170/236 (72%)	165 (97%)	5 (3%)	0	100	100
2	F	170/236 (72%)	165 (97%)	5 (3%)	0	100	100
3	G	126/130 (97%)	126 (100%)	0	0	100	100
3	H	126/130 (97%)	126 (100%)	0	0	100	100
3	I	126/130 (97%)	126 (100%)	0	0	100	100
4	J	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
4	K	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
4	L	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
All	All	2139/2454 (87%)	2104 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/306 (92%)	280 (100%)	0	100	100
1	C	280/306 (92%)	280 (100%)	0	100	100
1	D	280/306 (92%)	280 (100%)	0	100	100
2	B	145/194 (75%)	144 (99%)	1 (1%)	81	90
2	E	145/194 (75%)	144 (99%)	1 (1%)	81	90
2	F	145/194 (75%)	144 (99%)	1 (1%)	81	90
3	G	102/104 (98%)	102 (100%)	0	100	100
3	H	102/104 (98%)	102 (100%)	0	100	100
3	I	102/104 (98%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	91/93 (98%)	91 (100%)	0	100	100
4	K	91/93 (98%)	91 (100%)	0	100	100
4	L	91/93 (98%)	91 (100%)	0	100	100
All	All	1854/2091 (89%)	1851 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	143	LYS
2	E	143	LYS
2	F	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	56	HIS
1	C	18	HIS
2	E	47	GLN
2	E	146	ASN
1	D	18	HIS
2	F	47	GLN

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

39 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	5,1	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	M	2	5	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	N	1	6,1	14,14,15	0.78	1 (7%)	17,19,21	1.41	2 (11%)
6	NAG	N	2	6	14,14,15	0.29	0	17,19,21	0.80	1 (5%)
6	FUC	N	3	6	10,10,11	0.83	1 (10%)	14,14,16	1.13	1 (7%)
5	NAG	O	1	5,1	14,14,15	0.61	1 (7%)	17,19,21	0.56	0
5	NAG	O	2	5	14,14,15	0.40	0	17,19,21	0.49	0
7	NAG	P	1	7,1	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
7	NAG	P	2	7	14,14,15	0.26	0	17,19,21	0.80	1 (5%)
7	BMA	P	3	7	11,11,12	0.64	0	15,15,17	0.72	0
7	NAG	Q	1	7,1	14,14,15	0.47	0	17,19,21	1.09	2 (11%)
7	NAG	Q	2	7	14,14,15	0.46	0	17,19,21	0.48	0
7	BMA	Q	3	7	11,11,12	0.61	0	15,15,17	0.81	0
5	NAG	R	1	5,1	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	R	2	5	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	S	1	6,1	14,14,15	0.77	1 (7%)	17,19,21	1.42	2 (11%)
6	NAG	S	2	6	14,14,15	0.27	0	17,19,21	0.80	1 (5%)
6	FUC	S	3	6	10,10,11	0.82	1 (10%)	14,14,16	1.14	1 (7%)
5	NAG	T	1	5,1	14,14,15	0.60	1 (7%)	17,19,21	0.57	0
5	NAG	T	2	5	14,14,15	0.43	0	17,19,21	0.48	0
7	NAG	U	1	7,1	14,14,15	0.31	0	17,19,21	0.82	1 (5%)
7	NAG	U	2	7	14,14,15	0.24	0	17,19,21	0.80	1 (5%)
7	BMA	U	3	7	11,11,12	0.64	0	15,15,17	0.71	0
7	NAG	V	1	7,1	14,14,15	0.58	1 (7%)	17,19,21	1.05	2 (11%)
7	NAG	V	2	7	14,14,15	0.77	1 (7%)	17,19,21	0.79	1 (5%)
7	BMA	V	3	7	11,11,12	0.60	0	15,15,17	0.74	0
5	NAG	W	1	5,1	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	W	2	5	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	X	1	6,1	14,14,15	0.79	1 (7%)	17,19,21	1.41	2 (11%)
6	NAG	X	2	6	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
6	FUC	X	3	6	10,10,11	0.82	1 (10%)	14,14,16	1.14	1 (7%)
5	NAG	Y	1	5,1	14,14,15	0.57	0	17,19,21	0.57	0
5	NAG	Y	2	5	14,14,15	0.42	0	17,19,21	0.48	0
7	NAG	Z	1	7,1	14,14,15	0.31	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	Z	2	7	14,14,15	0.24	0	17,19,21	0.80	1 (5%)
7	BMA	Z	3	7	11,11,12	0.64	0	15,15,17	0.71	0
7	NAG	a	1	7,1	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
7	NAG	a	2	7	14,14,15	0.57	0	17,19,21	0.51	0
7	BMA	a	3	7	11,11,12	0.62	0	15,15,17	0.76	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
5	NAG	M	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
6	FUC	N	3	6	-	-	0/1/1/1
5	NAG	O	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
7	NAG	P	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
7	NAG	Q	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	4/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
6	FUC	S	3	6	-	-	0/1/1/1
5	NAG	T	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
7	NAG	U	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	U	2	7	-	2/6/23/26	0/1/1/1
7	BMA	U	3	7	-	1/2/19/22	0/1/1/1
7	NAG	V	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	V	2	7	-	3/6/23/26	0/1/1/1
7	BMA	V	3	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	W	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
6	NAG	X	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	X	2	6	-	4/6/23/26	0/1/1/1
6	FUC	X	3	6	-	-	0/1/1/1
5	NAG	Y	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
7	NAG	Z	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	1/2/19/22	0/1/1/1
7	NAG	a	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	a	2	7	-	4/6/23/26	0/1/1/1
7	BMA	a	3	7	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	1	NAG	O5-C1	2.84	1.48	1.43
6	N	1	NAG	O5-C1	2.83	1.48	1.43
6	S	1	NAG	O5-C1	2.79	1.48	1.43
7	V	2	NAG	O5-C1	2.31	1.47	1.43
6	N	3	FUC	C1-C2	2.24	1.57	1.52
6	X	3	FUC	C1-C2	2.23	1.57	1.52
6	S	3	FUC	C1-C2	2.23	1.57	1.52
5	O	1	NAG	C1-C2	2.04	1.55	1.52
7	V	1	NAG	C1-C2	2.00	1.55	1.52
5	T	1	NAG	C1-C2	2.00	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	1	NAG	C1-O5-C5	4.88	118.73	112.19
6	N	1	NAG	C1-O5-C5	4.84	118.67	112.19
6	X	1	NAG	C1-O5-C5	4.83	118.66	112.19
7	U	1	NAG	C2-N2-C7	2.88	126.76	122.90
7	P	1	NAG	C2-N2-C7	2.87	126.75	122.90
7	Z	1	NAG	C2-N2-C7	2.85	126.72	122.90
7	U	2	NAG	C2-N2-C7	2.75	126.58	122.90
6	N	2	NAG	C2-N2-C7	2.74	126.58	122.90
6	X	2	NAG	C2-N2-C7	2.73	126.56	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	2	NAG	C2-N2-C7	2.70	126.52	122.90
6	S	2	NAG	C2-N2-C7	2.69	126.51	122.90
7	Z	2	NAG	C2-N2-C7	2.69	126.51	122.90
6	S	1	NAG	C2-N2-C7	2.67	126.48	122.90
6	N	1	NAG	C2-N2-C7	2.65	126.45	122.90
6	X	1	NAG	C2-N2-C7	2.65	126.45	122.90
6	S	3	FUC	C1-O5-C5	2.65	119.21	112.97
6	N	3	FUC	C1-O5-C5	2.64	119.20	112.97
6	X	3	FUC	C1-O5-C5	2.64	119.19	112.97
7	Q	1	NAG	C1-O5-C5	2.36	115.35	112.19
7	V	1	NAG	C1-O5-C5	2.20	115.13	112.19
7	V	2	NAG	C1-C2-N2	2.20	113.89	110.43
7	a	1	NAG	C1-O5-C5	2.17	115.09	112.19
7	V	1	NAG	O4-C4-C5	2.11	114.51	109.32
7	Q	1	NAG	O4-C4-C3	-2.02	105.61	110.38

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	Q	2	NAG	C1-C2-N2-C7
7	V	2	NAG	C1-C2-N2-C7
7	a	2	NAG	C1-C2-N2-C7
7	Q	1	NAG	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
7	V	1	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
7	V	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	T	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
6	X	2	NAG	C8-C7-N2-C2
6	X	2	NAG	O7-C7-N2-C2
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
7	U	1	NAG	C8-C7-N2-C2
7	U	1	NAG	O7-C7-N2-C2
7	U	2	NAG	C8-C7-N2-C2
7	U	2	NAG	O7-C7-N2-C2
7	Z	1	NAG	C8-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	Z	2	NAG	C8-C7-N2-C2
7	Z	2	NAG	O7-C7-N2-C2
7	U	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
7	Q	2	NAG	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	S	2	NAG	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
5	R	1	NAG	C1-C2-N2-C7
5	W	1	NAG	C1-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7
5	O	1	NAG	C3-C2-N2-C7
5	R	1	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
5	Y	1	NAG	C3-C2-N2-C7
7	Q	1	NAG	C3-C2-N2-C7
7	Q	2	NAG	C3-C2-N2-C7
7	V	1	NAG	C3-C2-N2-C7
7	a	1	NAG	C3-C2-N2-C7
5	O	1	NAG	C1-C2-N2-C7
5	T	1	NAG	C1-C2-N2-C7
5	Y	1	NAG	C1-C2-N2-C7
7	Q	1	NAG	C1-C2-N2-C7
7	V	1	NAG	C1-C2-N2-C7
7	a	1	NAG	C1-C2-N2-C7
7	a	2	NAG	C3-C2-N2-C7
7	U	3	BMA	C4-C5-C6-O6
7	Z	3	BMA	C4-C5-C6-O6
7	P	3	BMA	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	1	NAG	2	0
5	T	2	NAG	1	0
7	V	2	NAG	4	0
7	Q	1	NAG	1	0
5	O	1	NAG	2	0
5	Y	1	NAG	2	0

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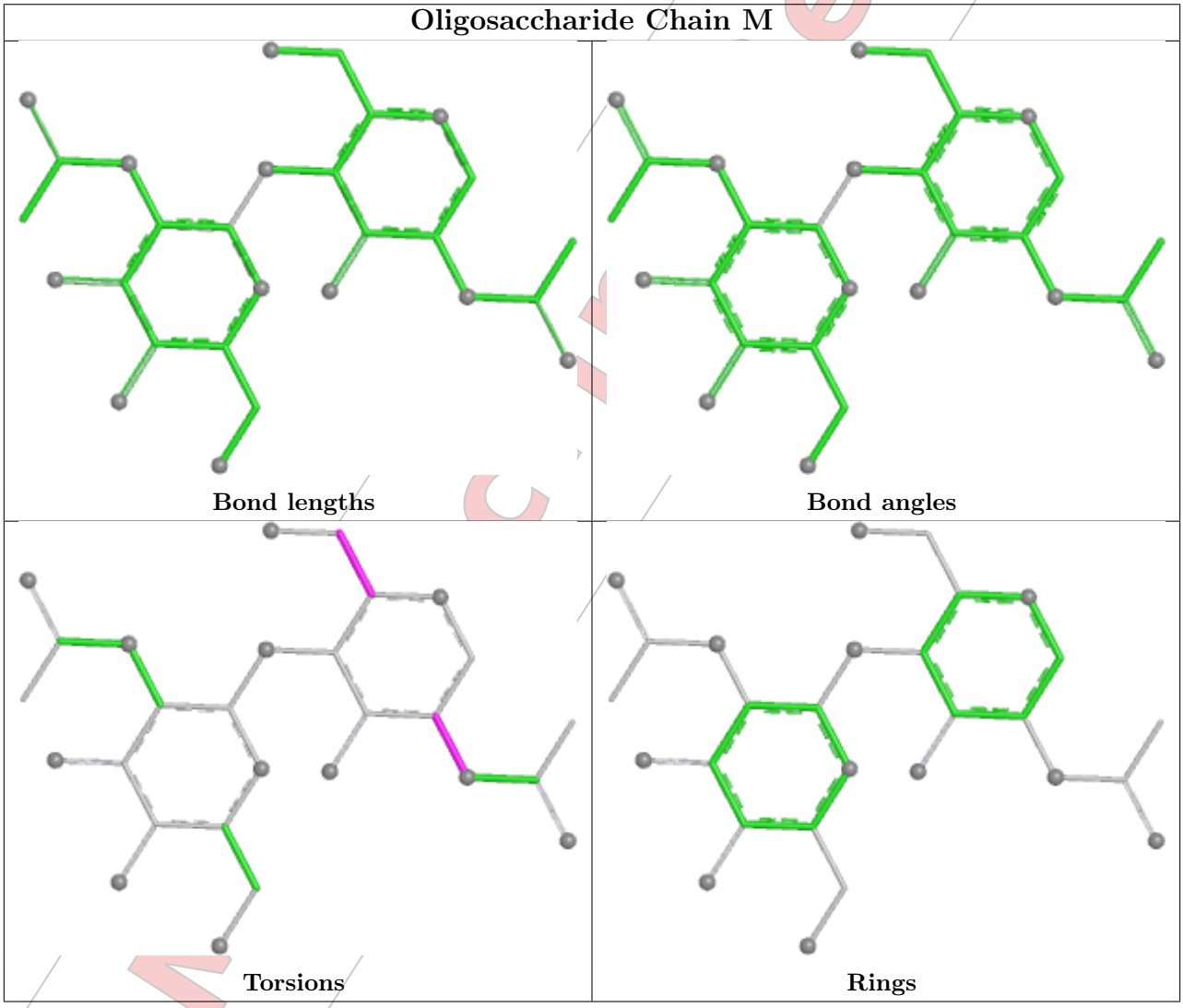
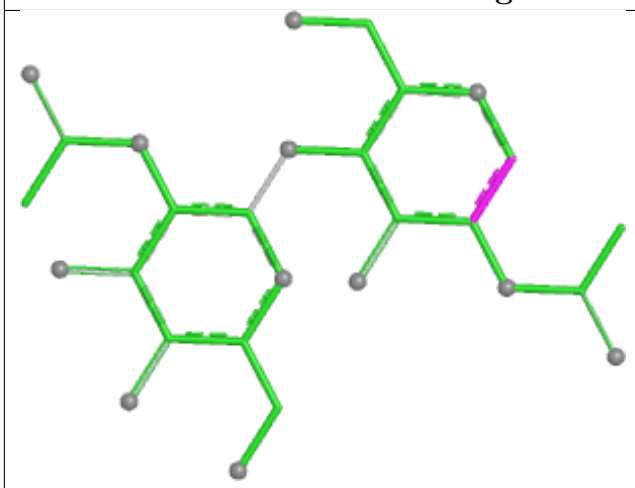
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	2	NAG	1	0
7	Q	2	NAG	2	0
5	O	2	NAG	1	0
7	V	1	NAG	1	0

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

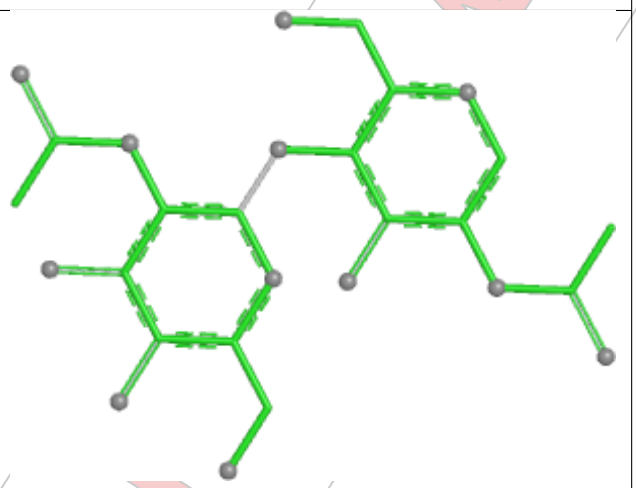
Oligosaccharide Chain M



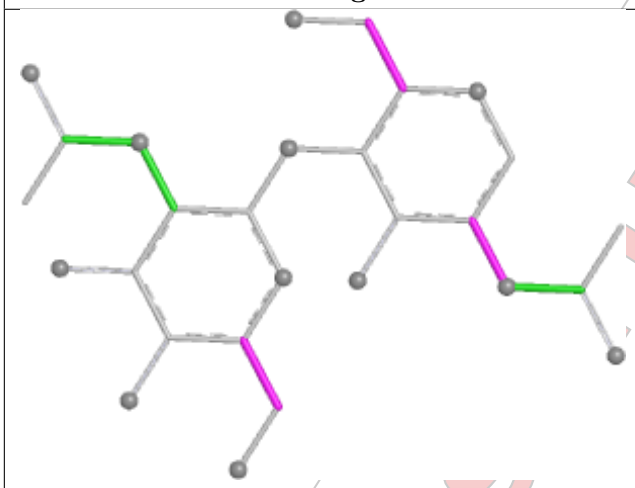
Oligosaccharide Chain O



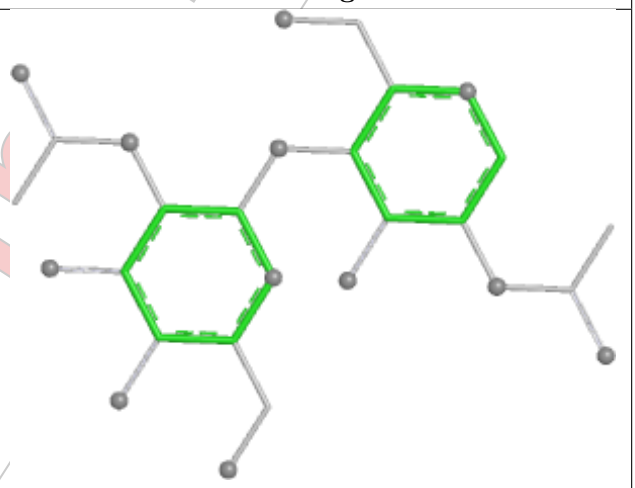
Bond lengths



Bond angles

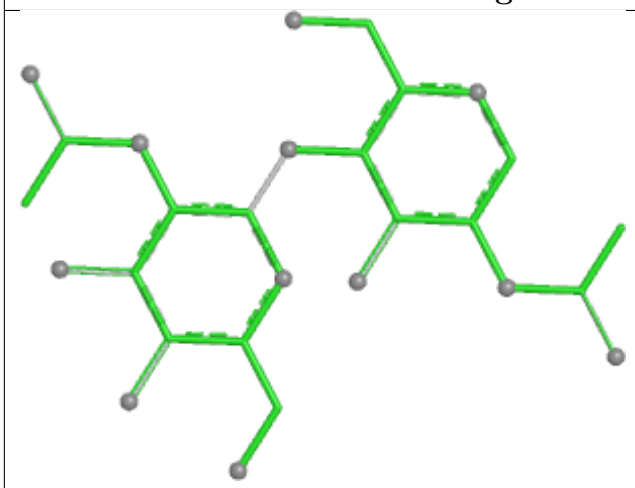


Torsions

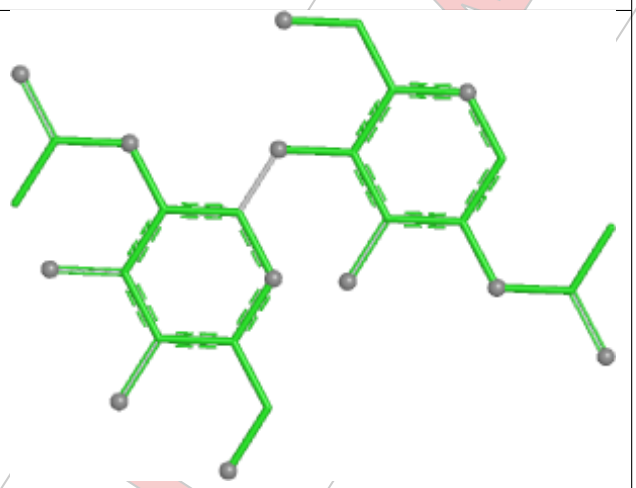


Rings

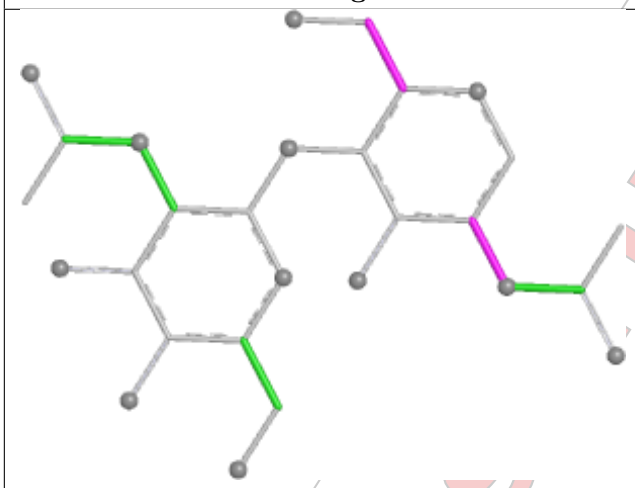
Oligosaccharide Chain R



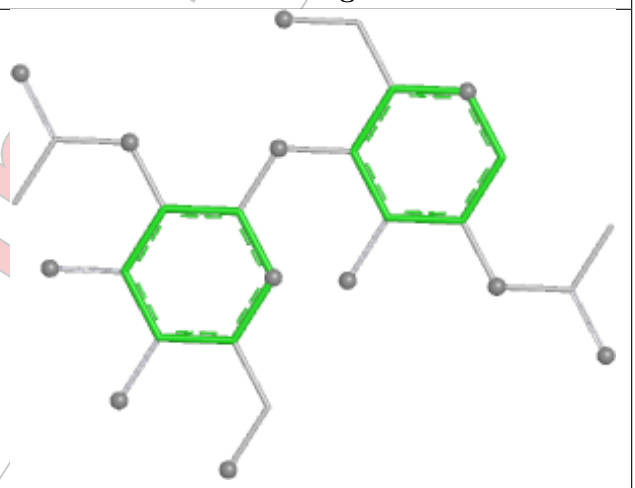
Bond lengths



Bond angles

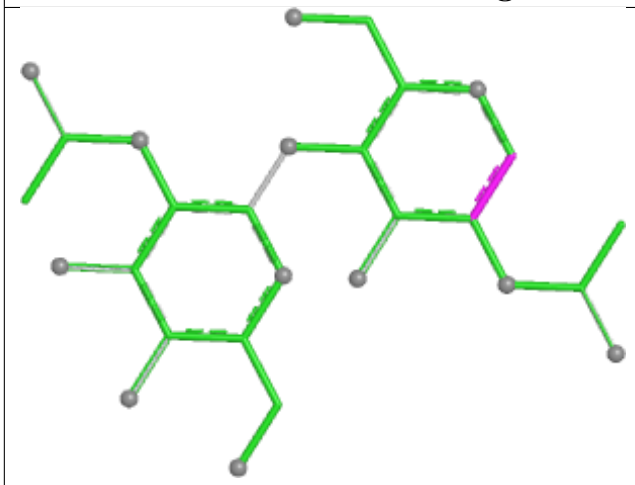


Torsions

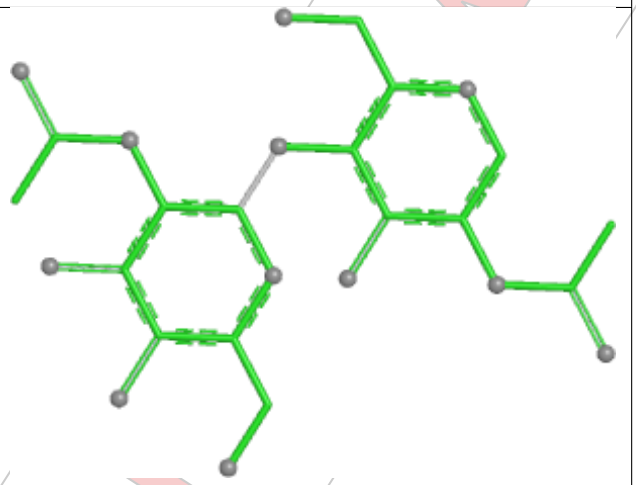


Rings

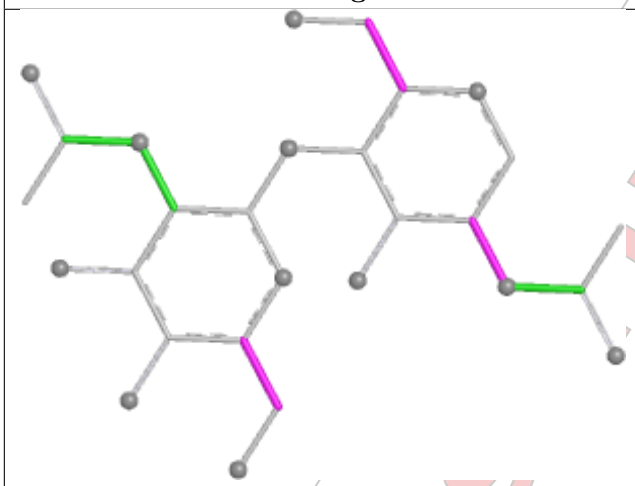
Oligosaccharide Chain T



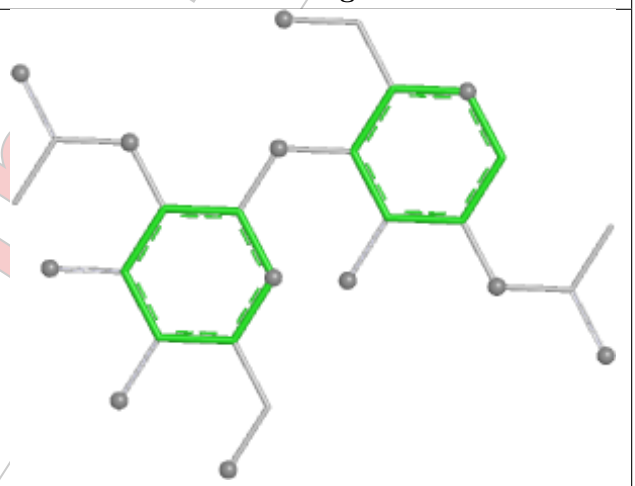
Bond lengths



Bond angles

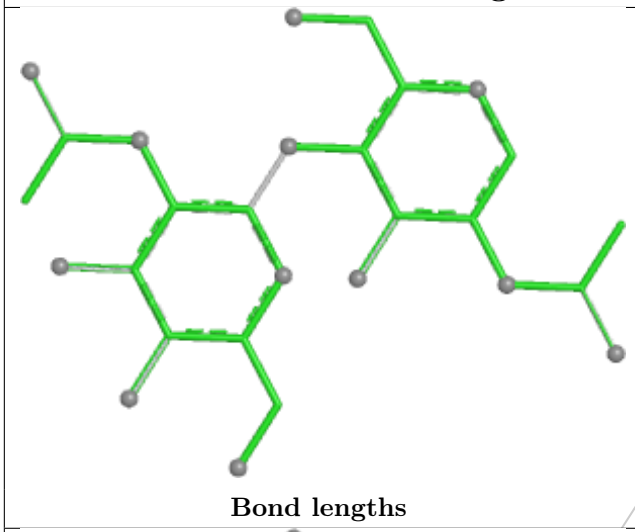


Torsions

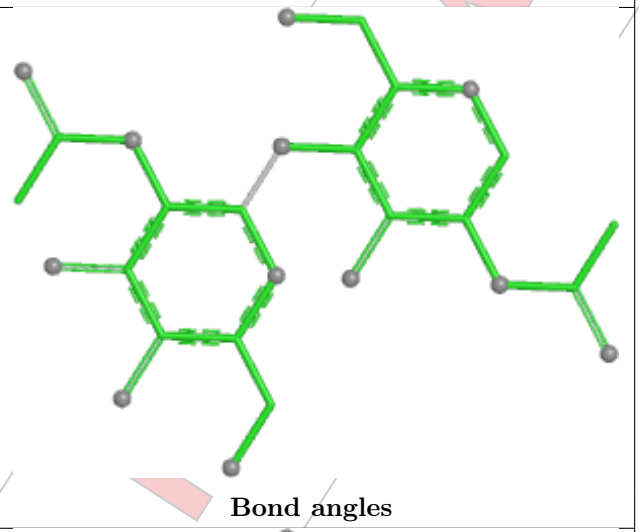


Rings

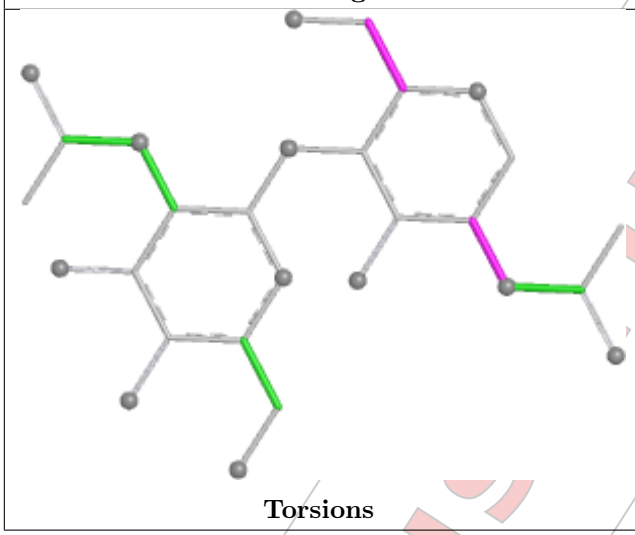
Oligosaccharide Chain W



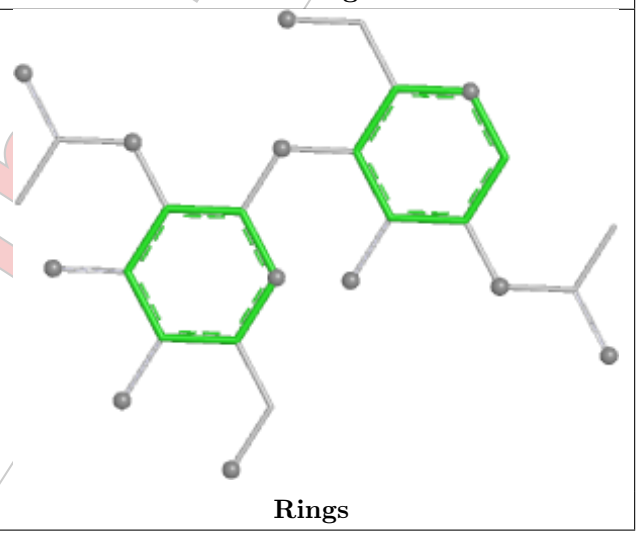
Bond lengths



Bond angles

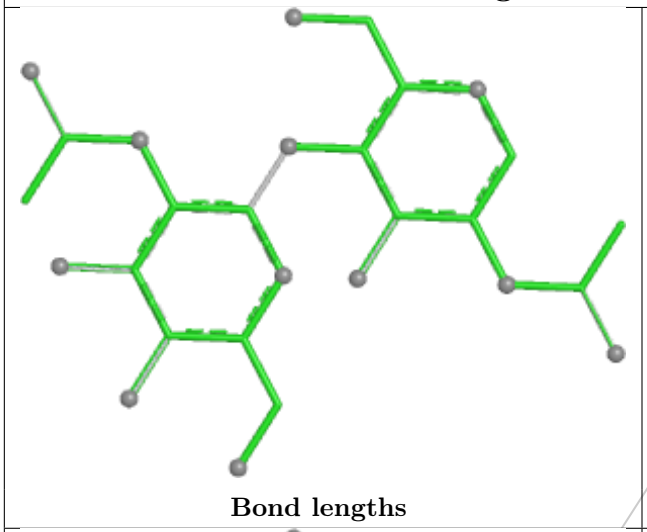


Torsions

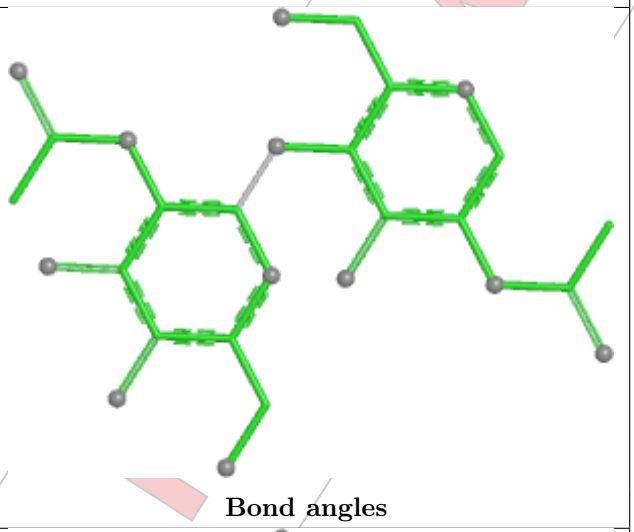


Rings

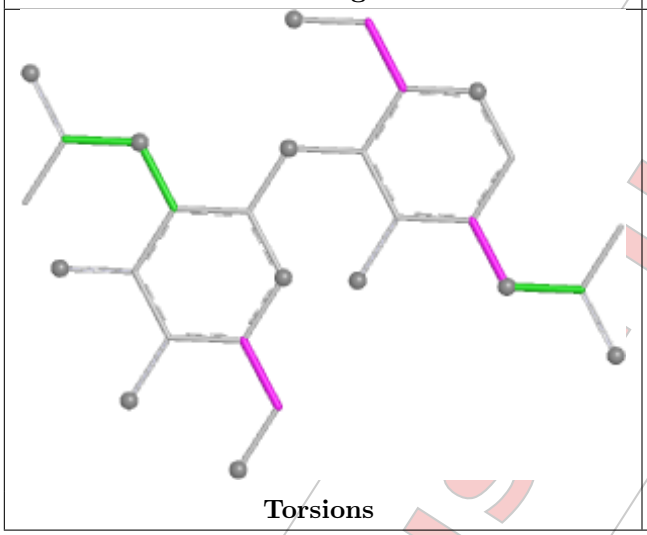
Oligosaccharide Chain Y



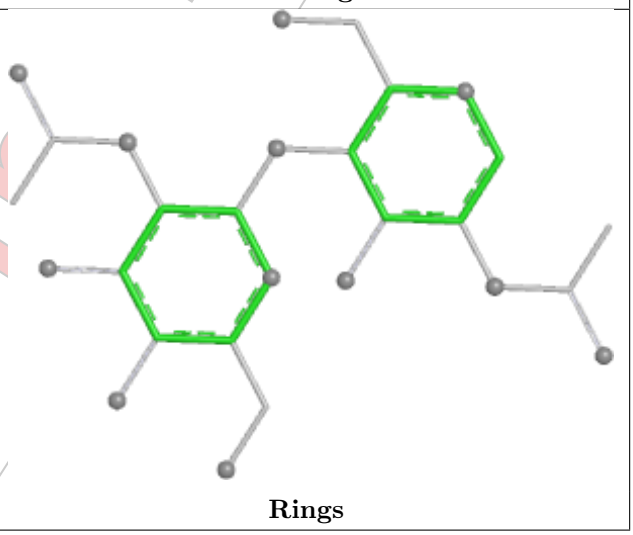
Bond lengths



Bond angles

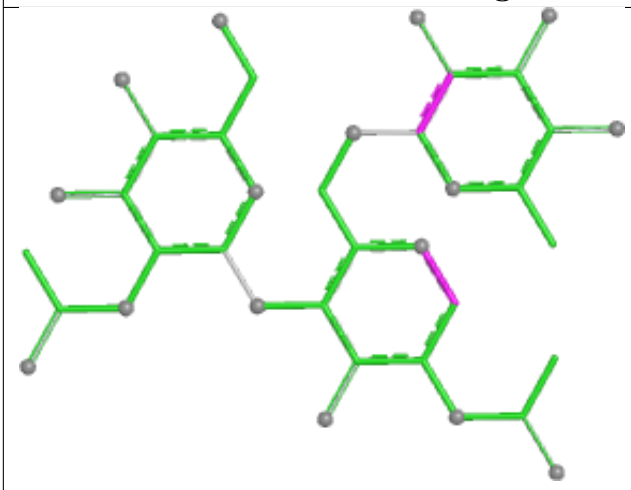


Torsions

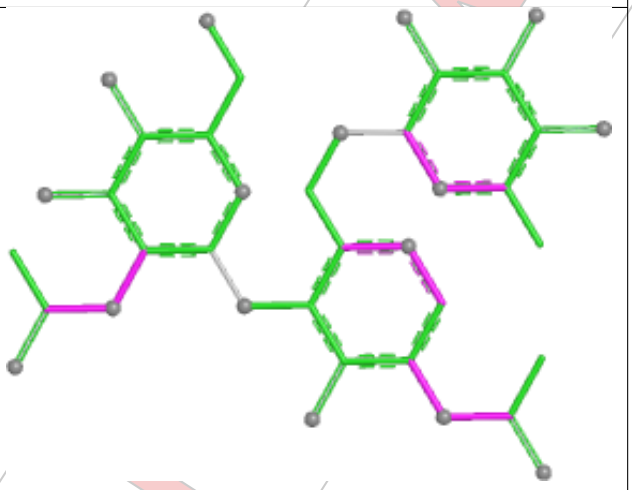


Rings

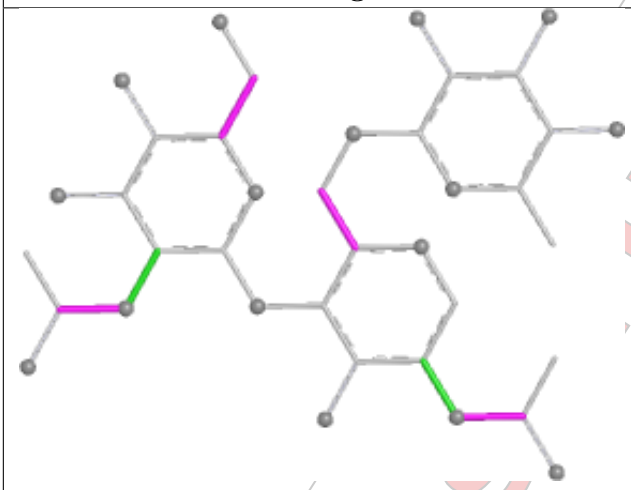
Oligosaccharide Chain N



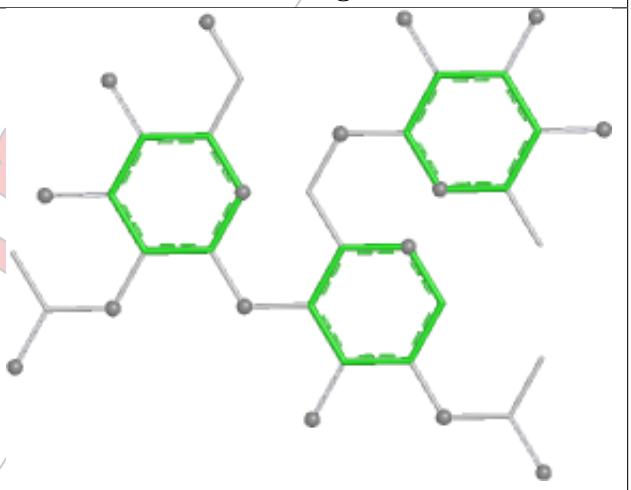
Bond lengths



Bond angles

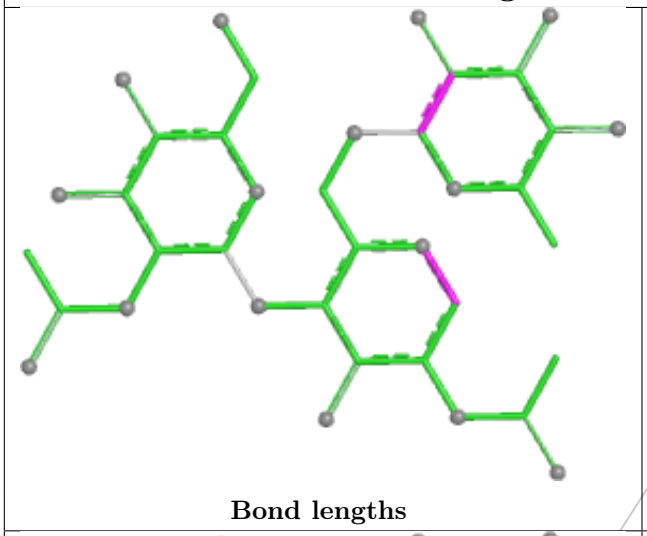


Torsions

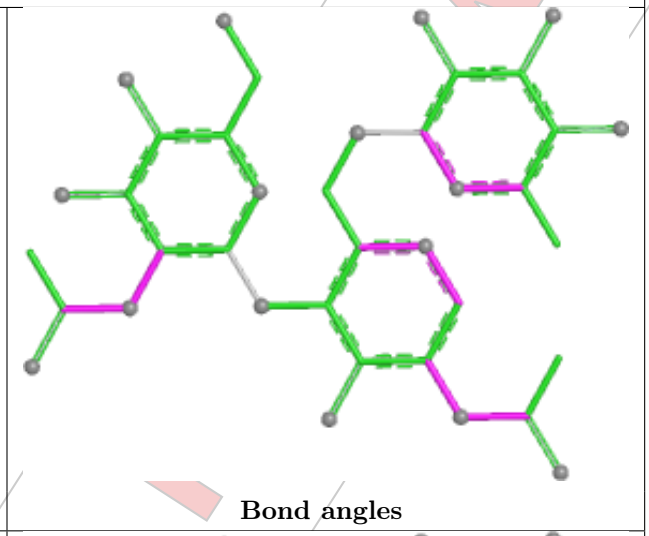


Rings

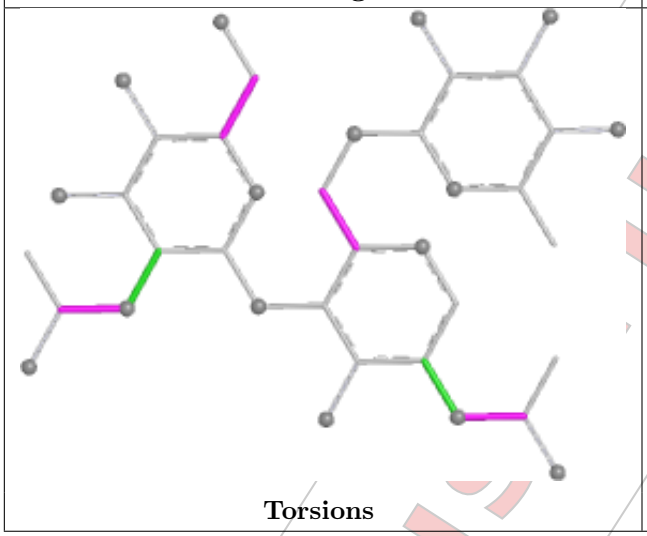
Oligosaccharide Chain S



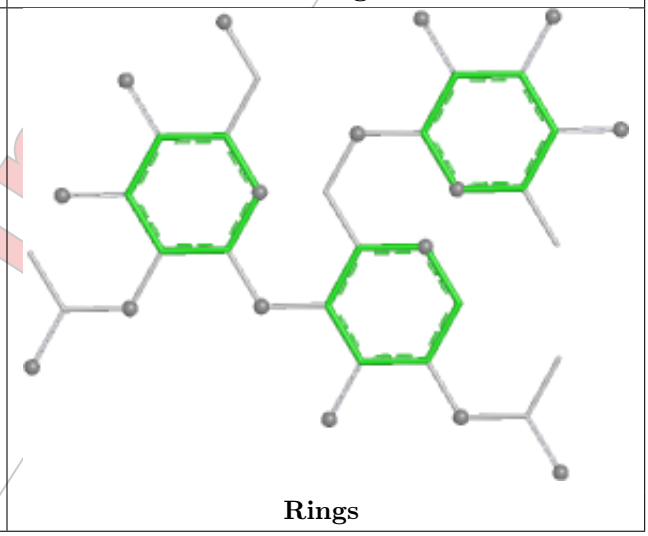
Bond lengths



Bond angles

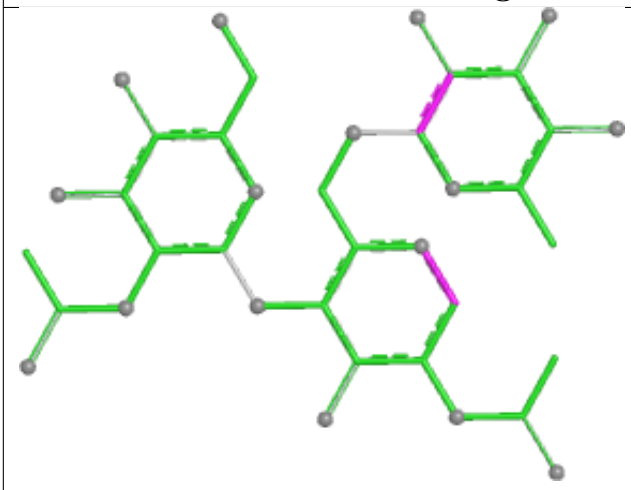


Torsions

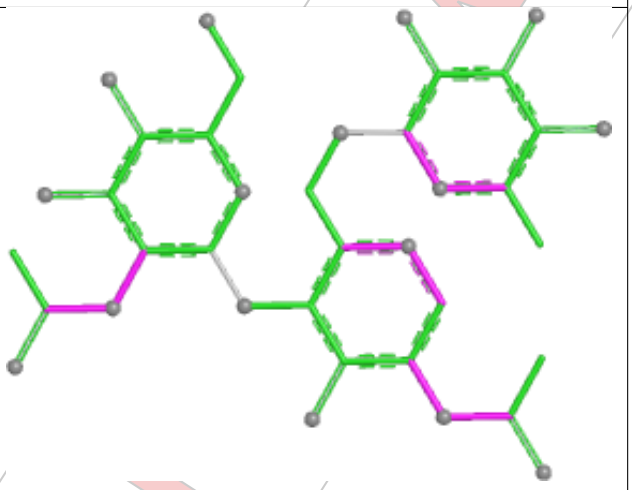


Rings

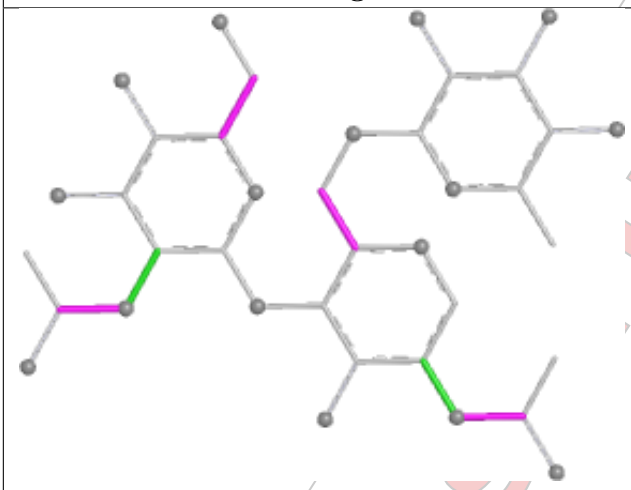
Oligosaccharide Chain X



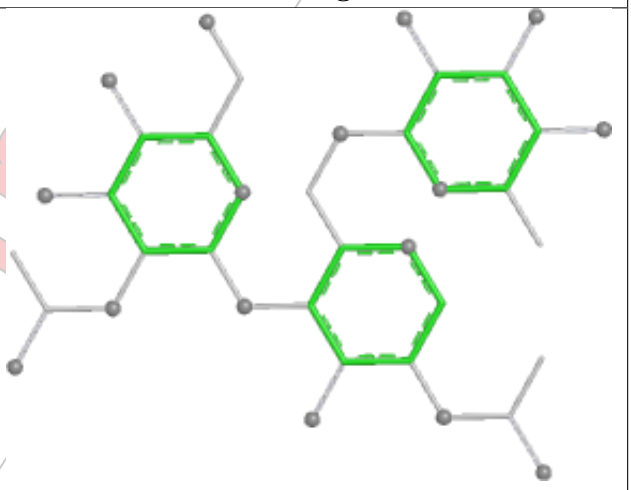
Bond lengths



Bond angles

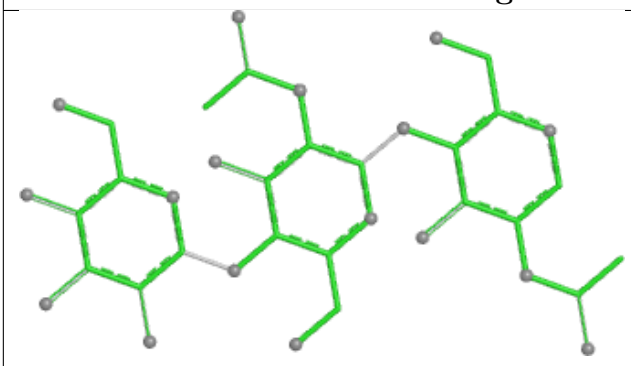


Torsions

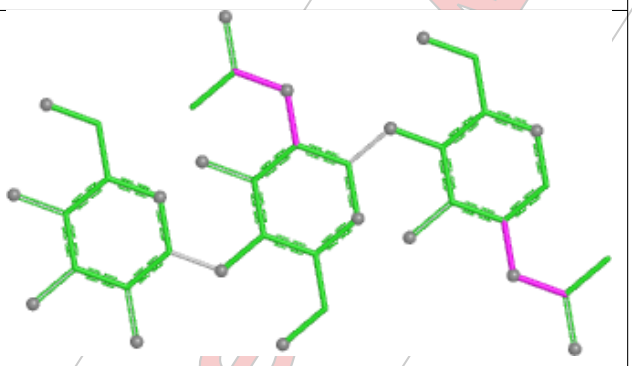


Rings

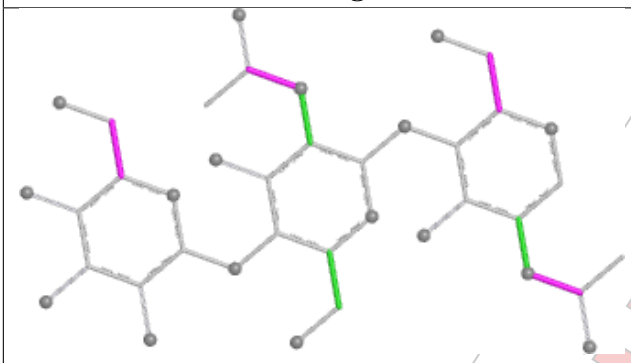
Oligosaccharide Chain P



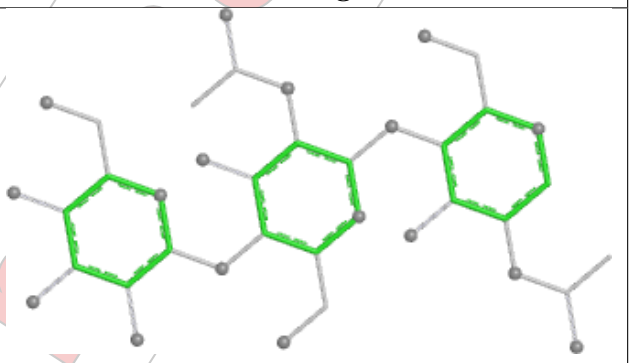
Bond lengths



Bond angles

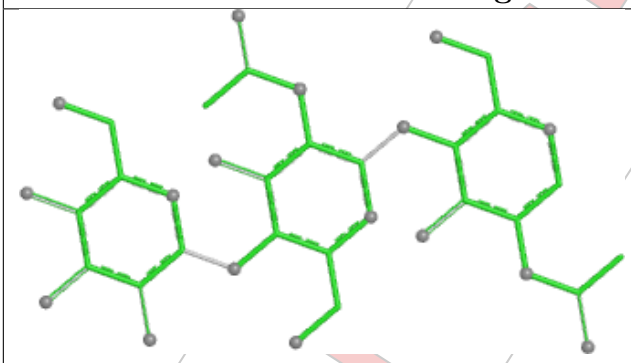


Torsions

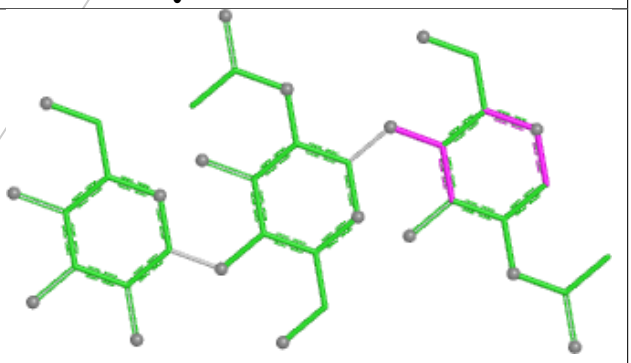


Rings

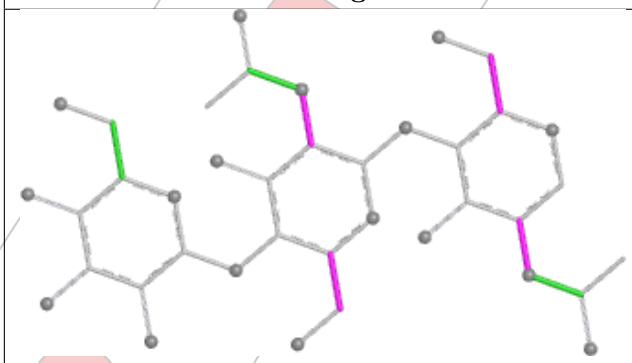
Oligosaccharide Chain Q



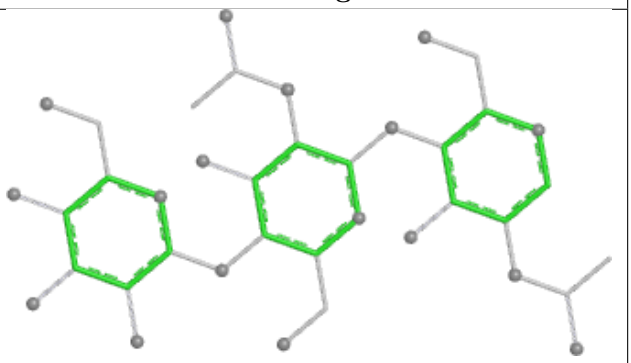
Bond lengths



Bond angles

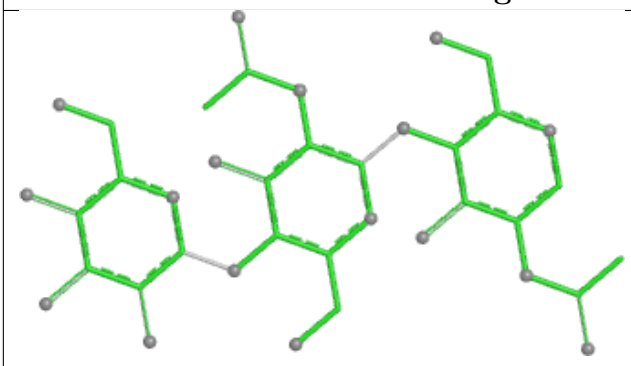


Torsions

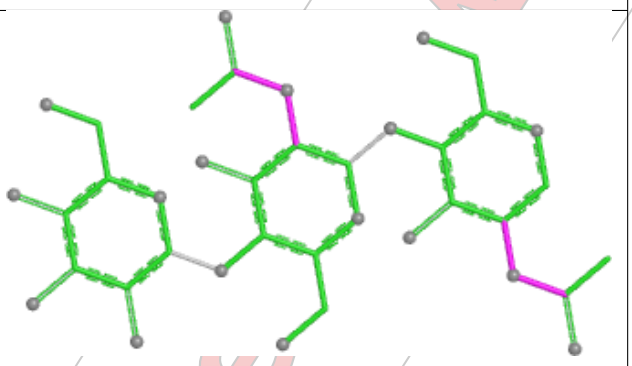


Rings

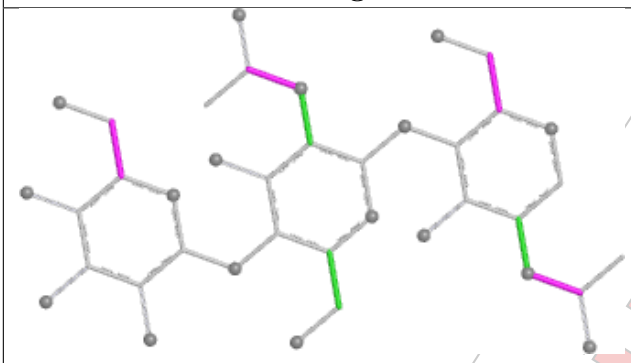
Oligosaccharide Chain U



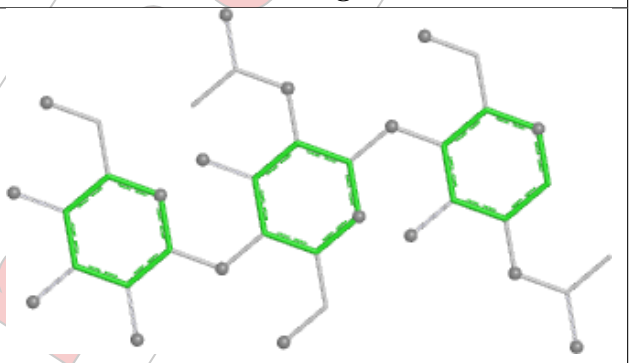
Bond lengths



Bond angles

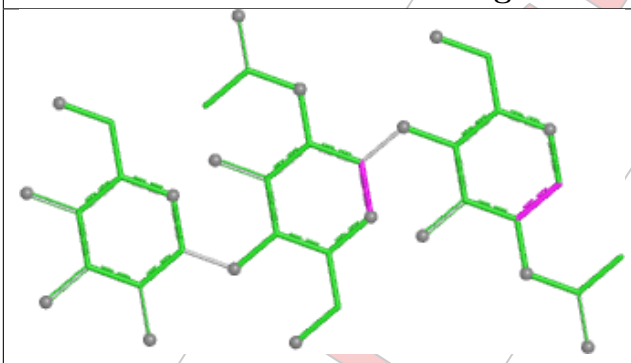


Torsions

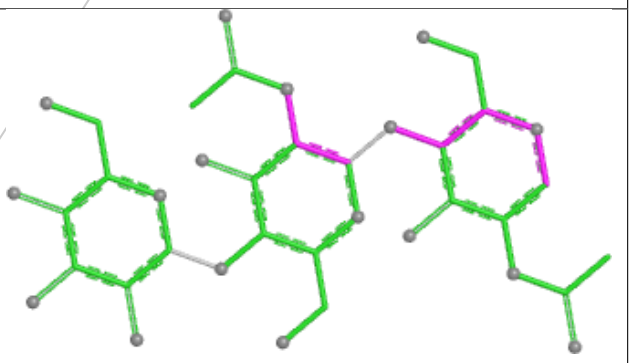


Rings

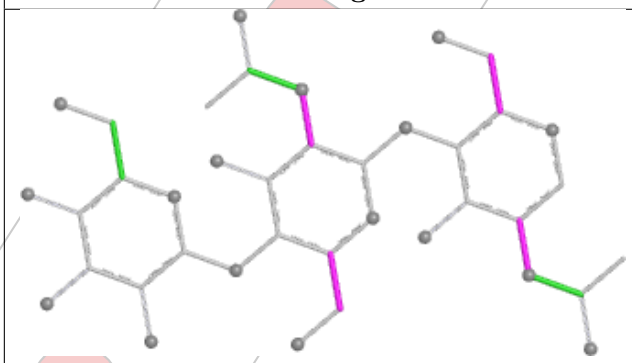
Oligosaccharide Chain V



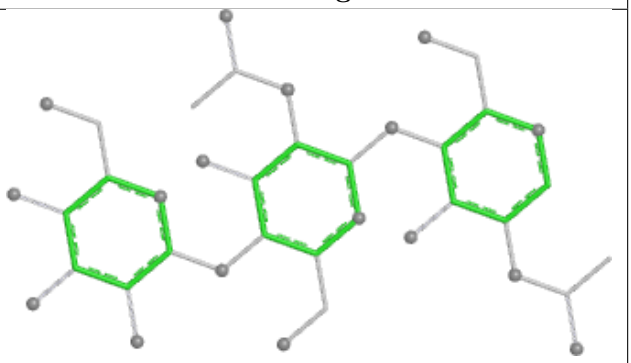
Bond lengths



Bond angles

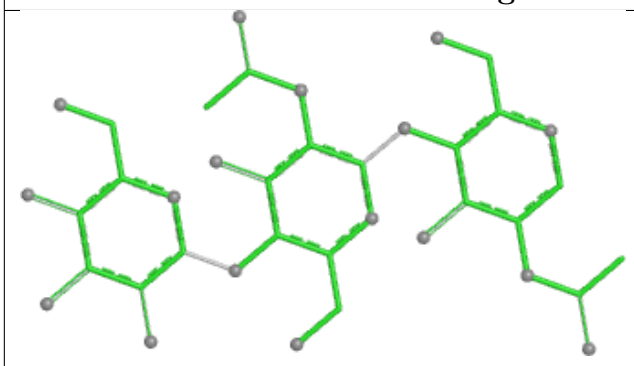


Torsions

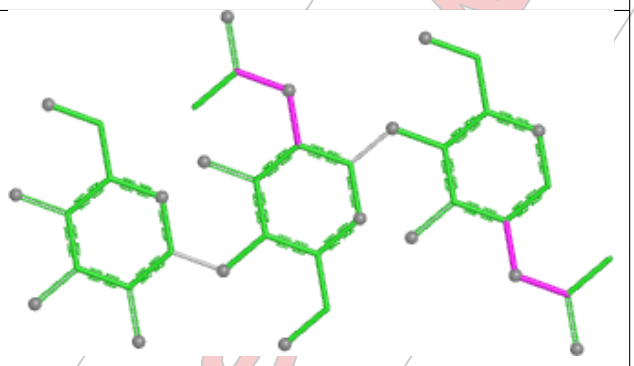


Rings

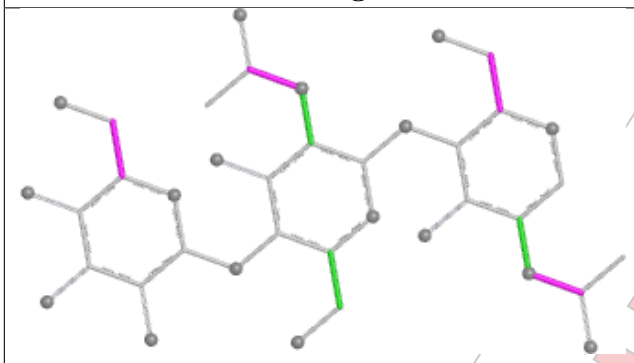
Oligosaccharide Chain Z



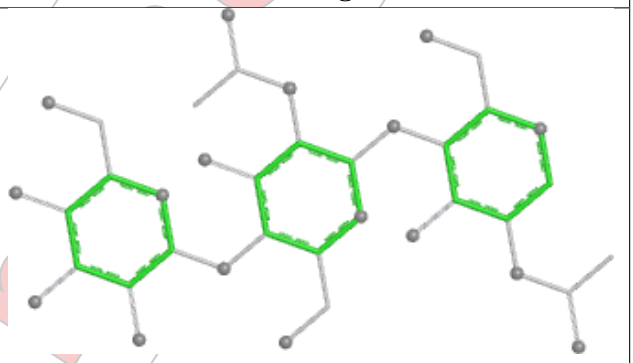
Bond lengths



Bond angles

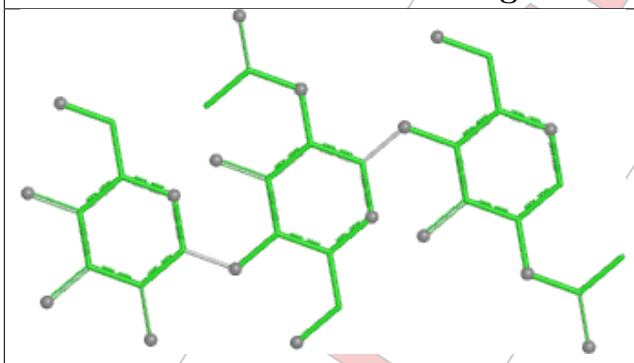


Torsions

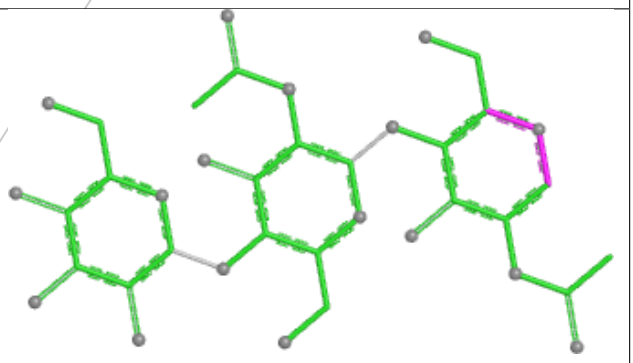


Rings

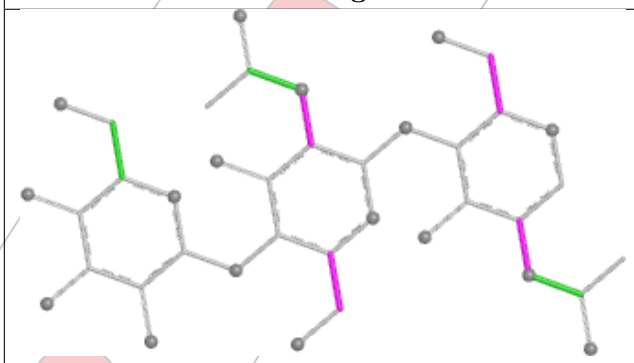
Oligosaccharide Chain a



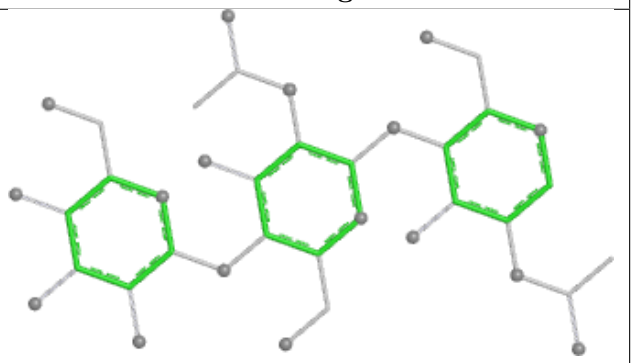
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

18 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	404	1	14,14,15	0.23	0	17,19,21	0.43	0
8	NAG	D	403	1	14,14,15	0.26	0	17,19,21	0.47	0
8	NAG	C	404	1	14,14,15	0.25	0	17,19,21	0.44	0
8	NAG	C	405	1	14,14,15	0.29	0	17,19,21	0.77	1 (5%)
8	NAG	B	301	2	14,14,15	0.22	0	17,19,21	0.52	0
8	NAG	D	405	1	14,14,15	0.28	0	17,19,21	0.76	1 (5%)
8	NAG	A	405	1	14,14,15	0.31	0	17,19,21	0.77	1 (5%)
8	NAG	E	301	2	14,14,15	0.22	0	17,19,21	0.53	0
8	NAG	A	402	1	14,14,15	0.31	0	17,19,21	0.46	0
8	NAG	A	403	1	14,14,15	0.26	0	17,19,21	0.47	0
8	NAG	C	402	1	14,14,15	0.32	0	17,19,21	0.46	0
8	NAG	D	404	1	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	C	401	1	14,14,15	0.29	0	17,19,21	0.45	0
8	NAG	D	402	1	14,14,15	0.32	0	17,19,21	0.47	0
8	NAG	A	401	1	14,14,15	0.29	0	17,19,21	0.44	0
8	NAG	F	301	2	14,14,15	0.21	0	17,19,21	0.52	0
8	NAG	D	401	1	14,14,15	0.28	0	17,19,21	0.45	0
8	NAG	C	403	1	14,14,15	0.25	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	404	1	-	2/6/23/26	0/1/1/1
8	NAG	D	403	1	-	2/6/23/26	0/1/1/1
8	NAG	C	404	1	-	2/6/23/26	0/1/1/1
8	NAG	C	405	1	-	2/6/23/26	0/1/1/1
8	NAG	B	301	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	405	1	-	2/6/23/26	0/1/1/1
8	NAG	A	405	1	-	2/6/23/26	0/1/1/1
8	NAG	E	301	2	-	2/6/23/26	0/1/1/1
8	NAG	A	402	1	-	2/6/23/26	0/1/1/1
8	NAG	A	403	1	-	3/6/23/26	0/1/1/1
8	NAG	C	402	1	-	2/6/23/26	0/1/1/1
8	NAG	D	404	1	-	2/6/23/26	0/1/1/1
8	NAG	C	401	1	-	2/6/23/26	0/1/1/1
8	NAG	D	402	1	-	2/6/23/26	0/1/1/1
8	NAG	A	401	1	-	2/6/23/26	0/1/1/1
8	NAG	F	301	2	-	2/6/23/26	0/1/1/1
8	NAG	D	401	1	-	2/6/23/26	0/1/1/1
8	NAG	C	403	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	405	NAG	C2-N2-C7	2.62	126.41	122.90
8	A	405	NAG	C2-N2-C7	2.61	126.40	122.90
8	D	405	NAG	C2-N2-C7	2.58	126.36	122.90

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	301	NAG	C4-C5-C6-O6
8	E	301	NAG	C4-C5-C6-O6
8	F	301	NAG	C4-C5-C6-O6
8	A	403	NAG	C4-C5-C6-O6
8	A	404	NAG	C4-C5-C6-O6
8	C	403	NAG	C4-C5-C6-O6
8	C	404	NAG	C4-C5-C6-O6
8	D	403	NAG	C4-C5-C6-O6
8	D	404	NAG	C4-C5-C6-O6
8	A	402	NAG	O5-C5-C6-O6
8	C	402	NAG	O5-C5-C6-O6
8	D	402	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	402	NAG	C4-C5-C6-O6
8	C	402	NAG	C4-C5-C6-O6
8	D	402	NAG	C4-C5-C6-O6
8	B	301	NAG	O5-C5-C6-O6
8	E	301	NAG	O5-C5-C6-O6
8	F	301	NAG	O5-C5-C6-O6
8	A	404	NAG	O5-C5-C6-O6
8	C	404	NAG	O5-C5-C6-O6
8	D	404	NAG	O5-C5-C6-O6
8	A	403	NAG	O5-C5-C6-O6
8	C	403	NAG	O5-C5-C6-O6
8	D	403	NAG	O5-C5-C6-O6
8	A	405	NAG	C8-C7-N2-C2
8	A	405	NAG	O7-C7-N2-C2
8	C	405	NAG	C8-C7-N2-C2
8	C	405	NAG	O7-C7-N2-C2
8	D	405	NAG	C8-C7-N2-C2
8	D	405	NAG	O7-C7-N2-C2
8	A	401	NAG	O5-C5-C6-O6
8	C	401	NAG	O5-C5-C6-O6
8	D	401	NAG	O5-C5-C6-O6
8	A	401	NAG	C4-C5-C6-O6
8	C	401	NAG	C4-C5-C6-O6
8	D	401	NAG	C4-C5-C6-O6
8	A	403	NAG	C1-C2-N2-C7
8	C	403	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

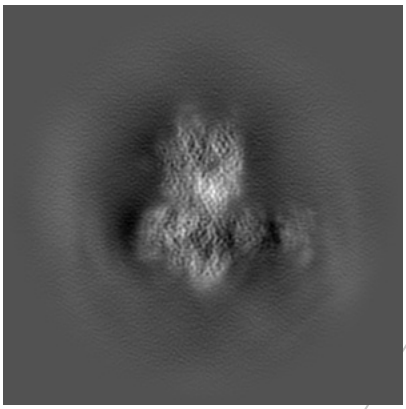
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70235. These allow visual inspection of the internal detail of the map and identification of artifacts.

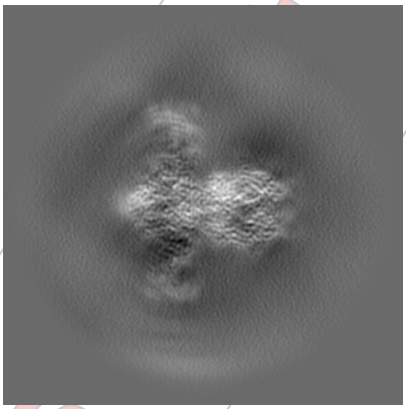
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

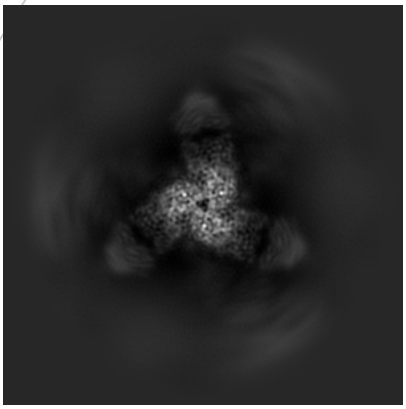
6.1.1 Primary map



X

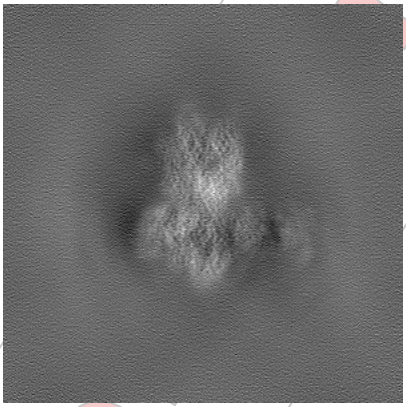


Y

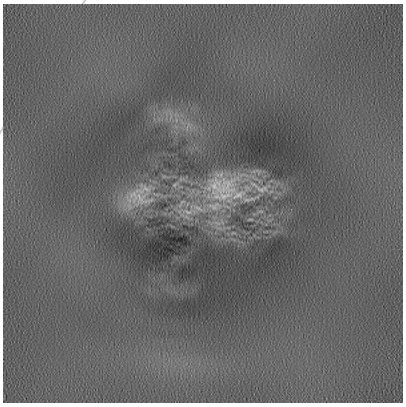


Z

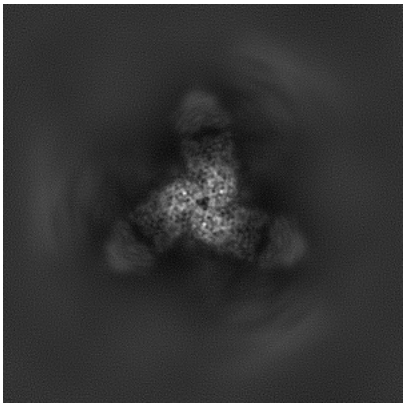
6.1.2 Raw map



X



Y

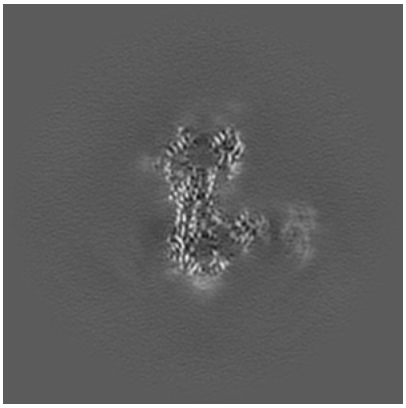


Z

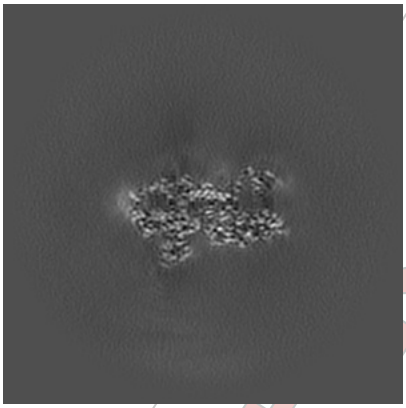
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

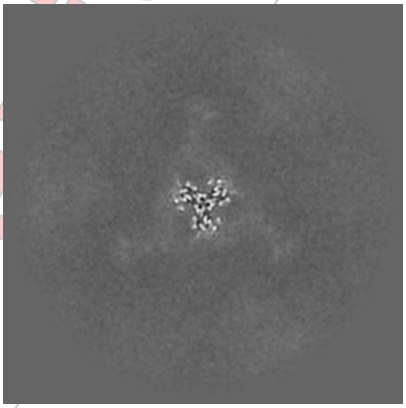
6.2.1 Primary map



X Index: 220

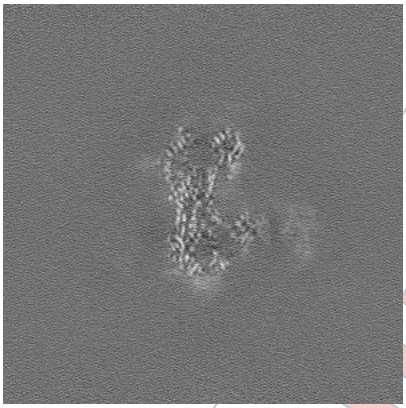


Y Index: 220

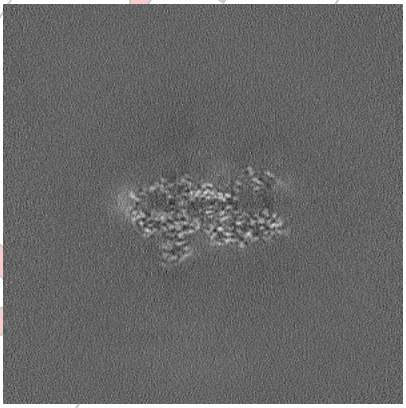


Z Index: 220

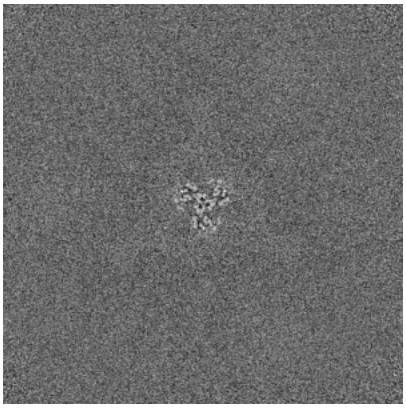
6.2.2 Raw map



X Index: 220



Y Index: 220

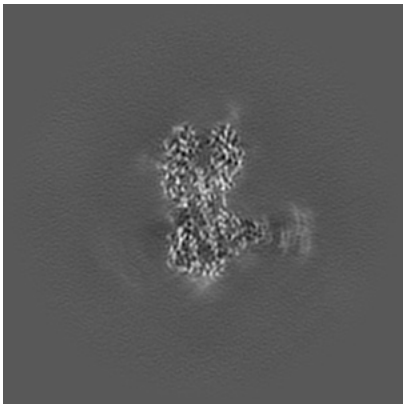


Z Index: 220

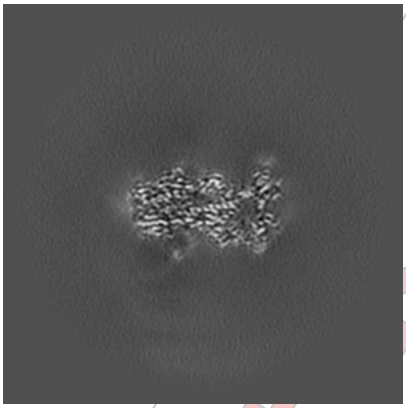
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

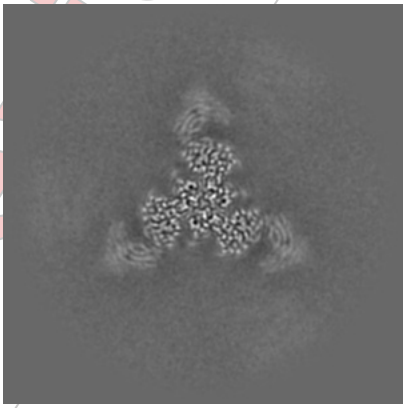
6.3.1 Primary map



X Index: 227

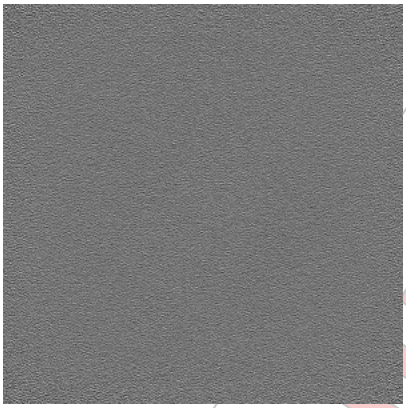


Y Index: 231

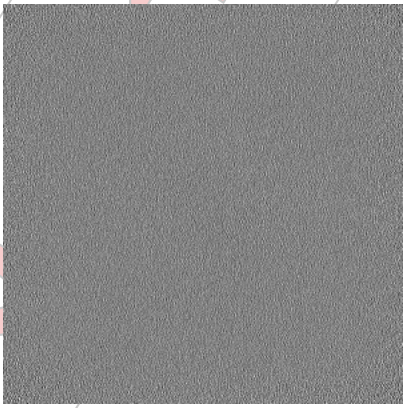


Z Index: 197

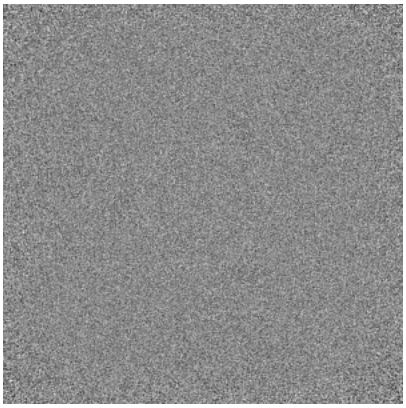
6.3.2 Raw map



X Index: 0



Y Index: 0

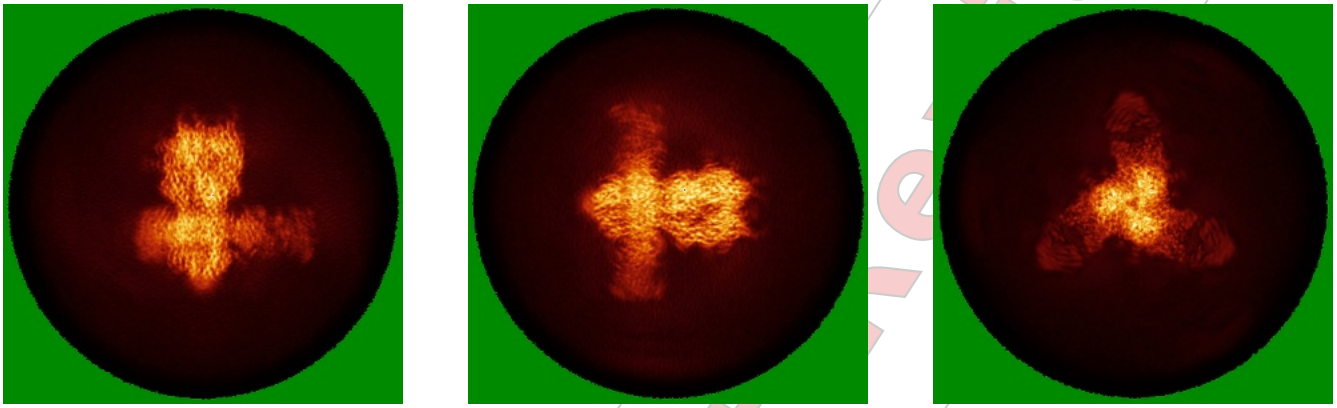


Z Index: 0

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

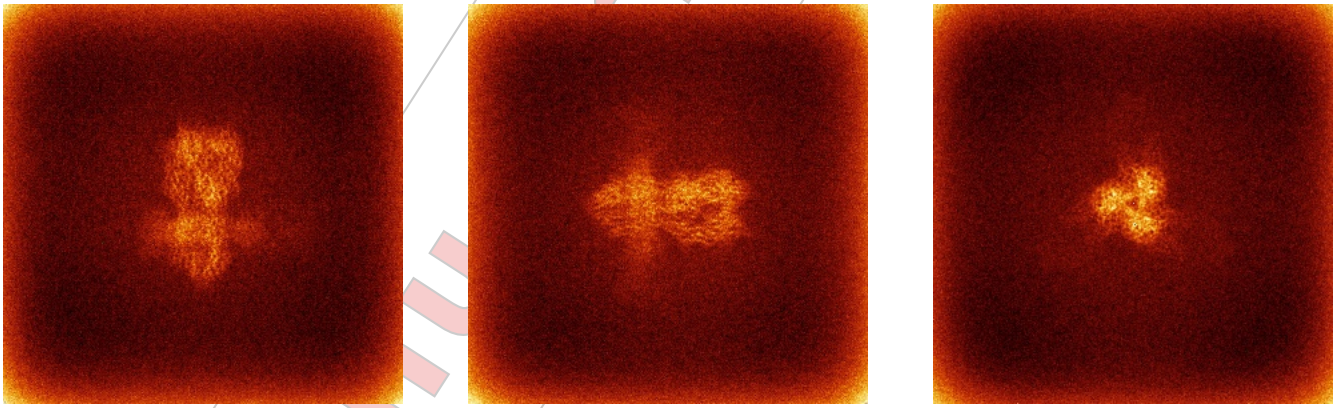
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

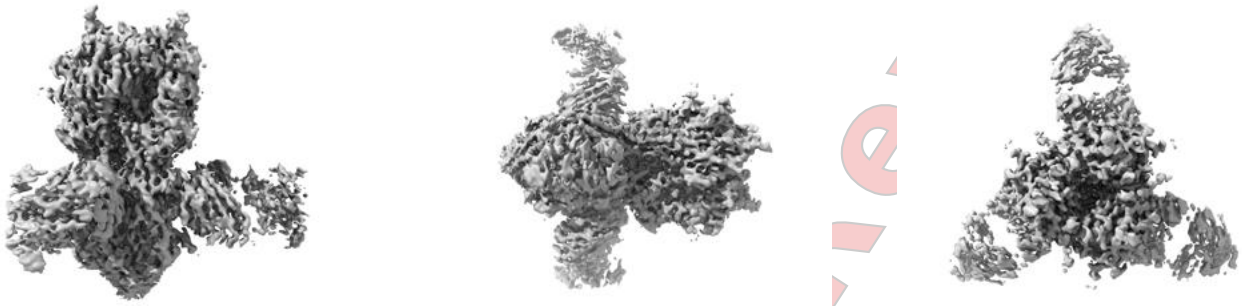


X Y Z

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)

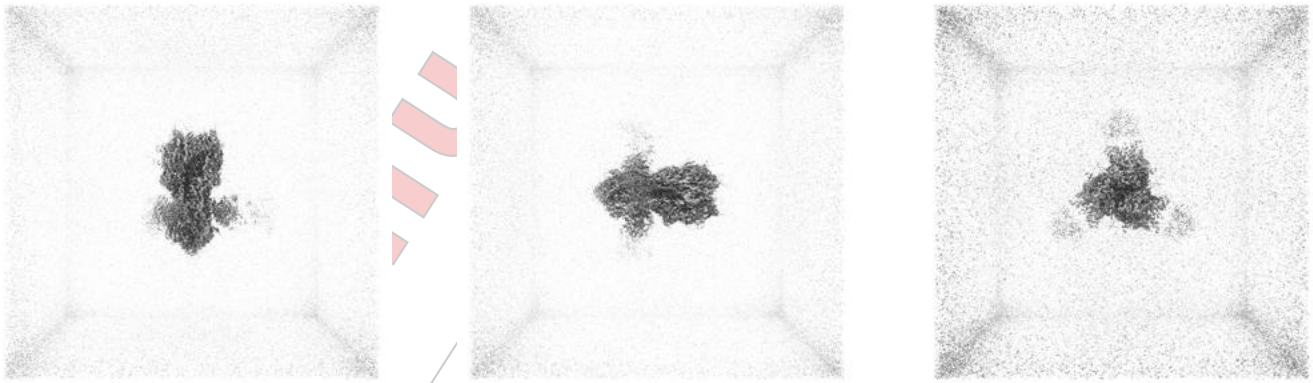
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

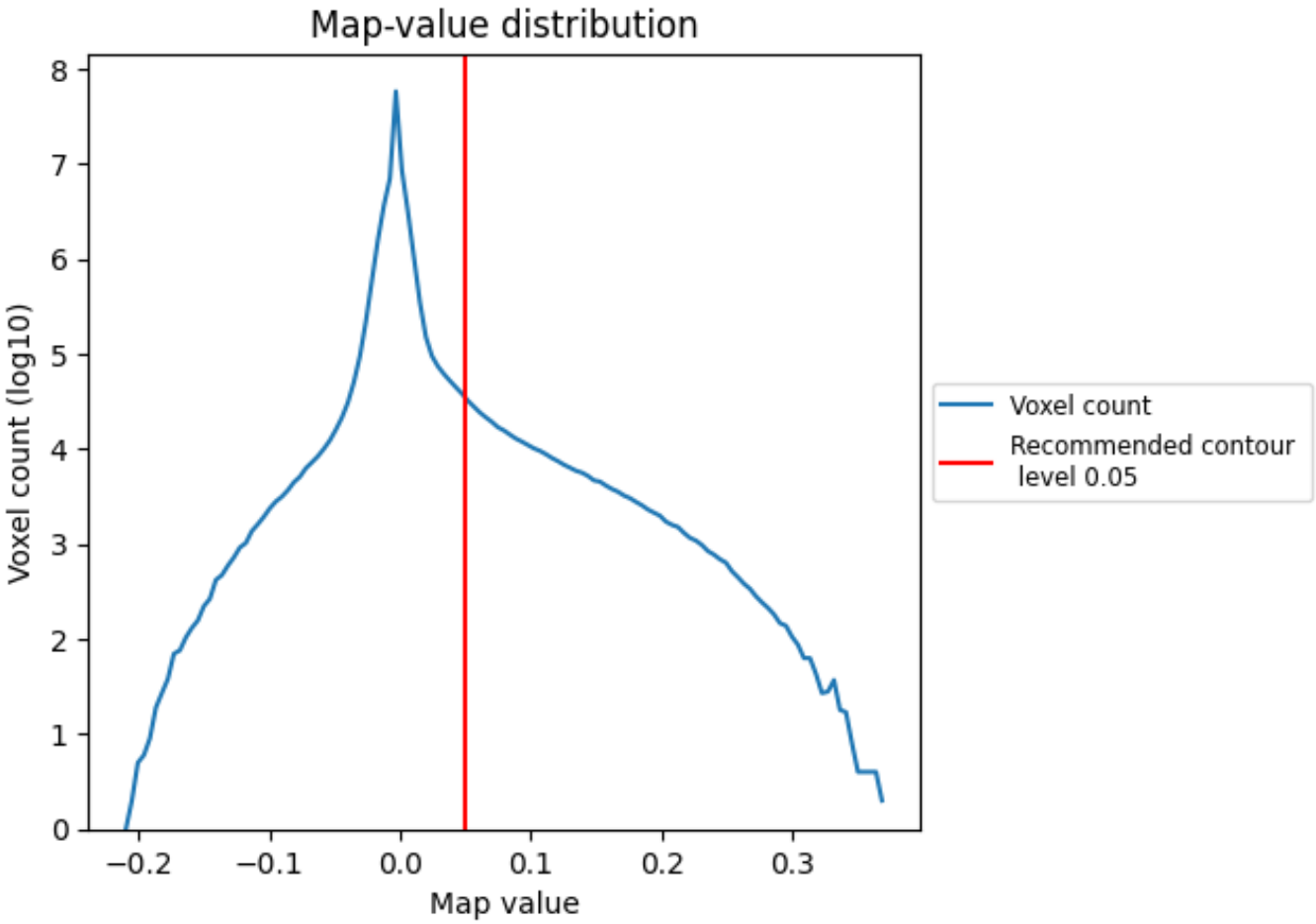
6.6 Mask visualisation (i)

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

7 Map analysis

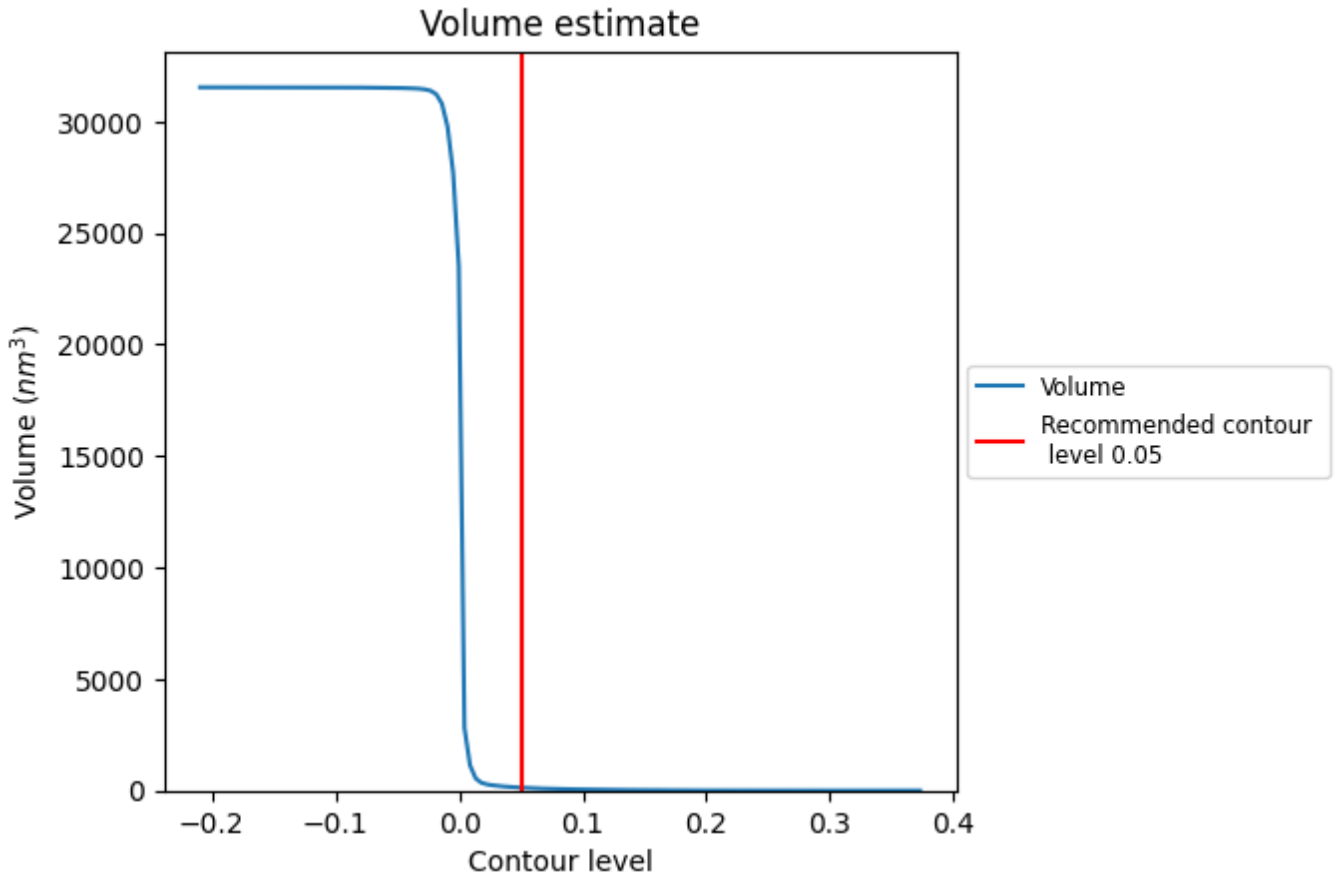
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

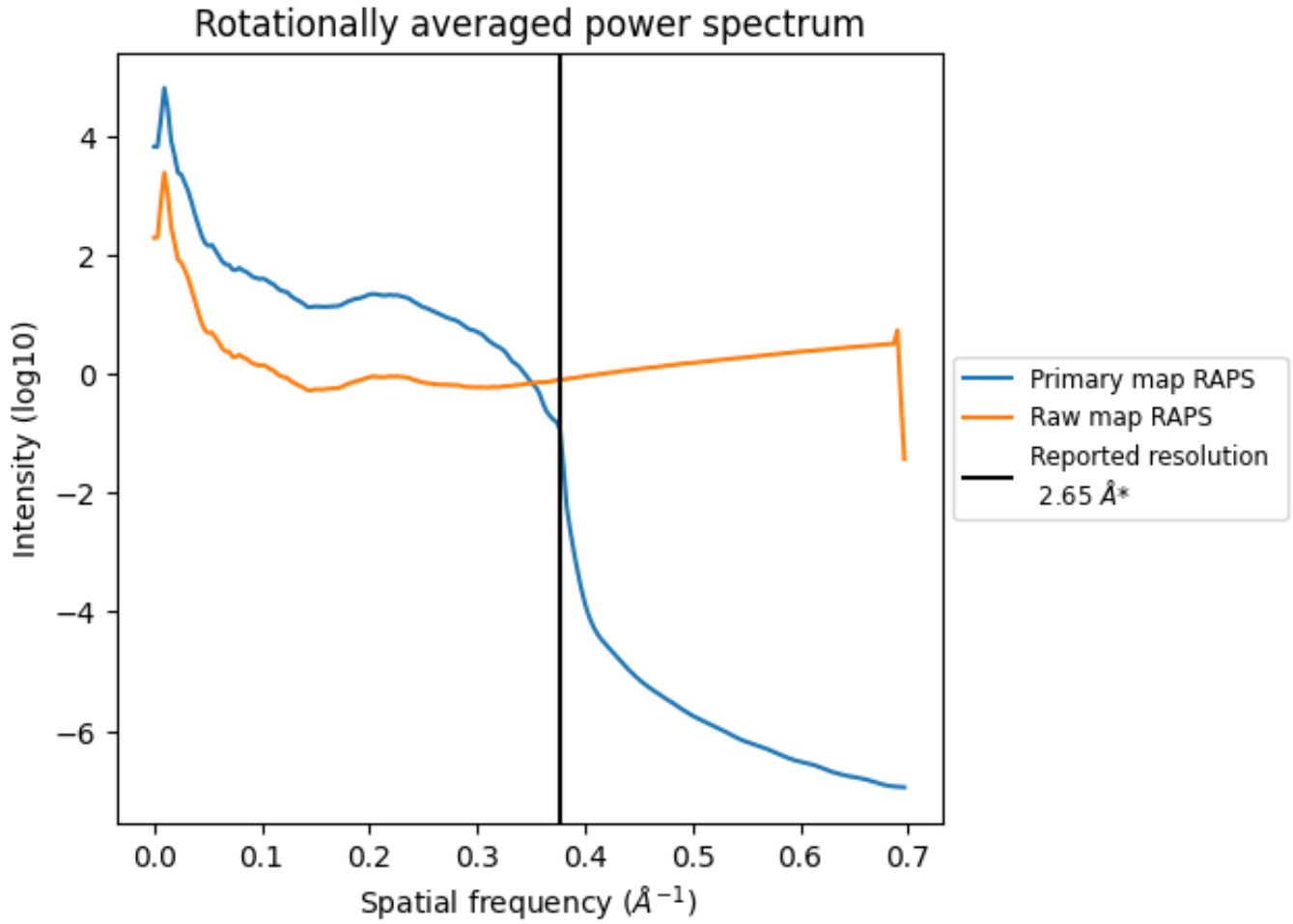
7.2 Volume estimate



The volume at the recommended contour level is 130 nm^3; this corresponds to an approximate mass of 117 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)

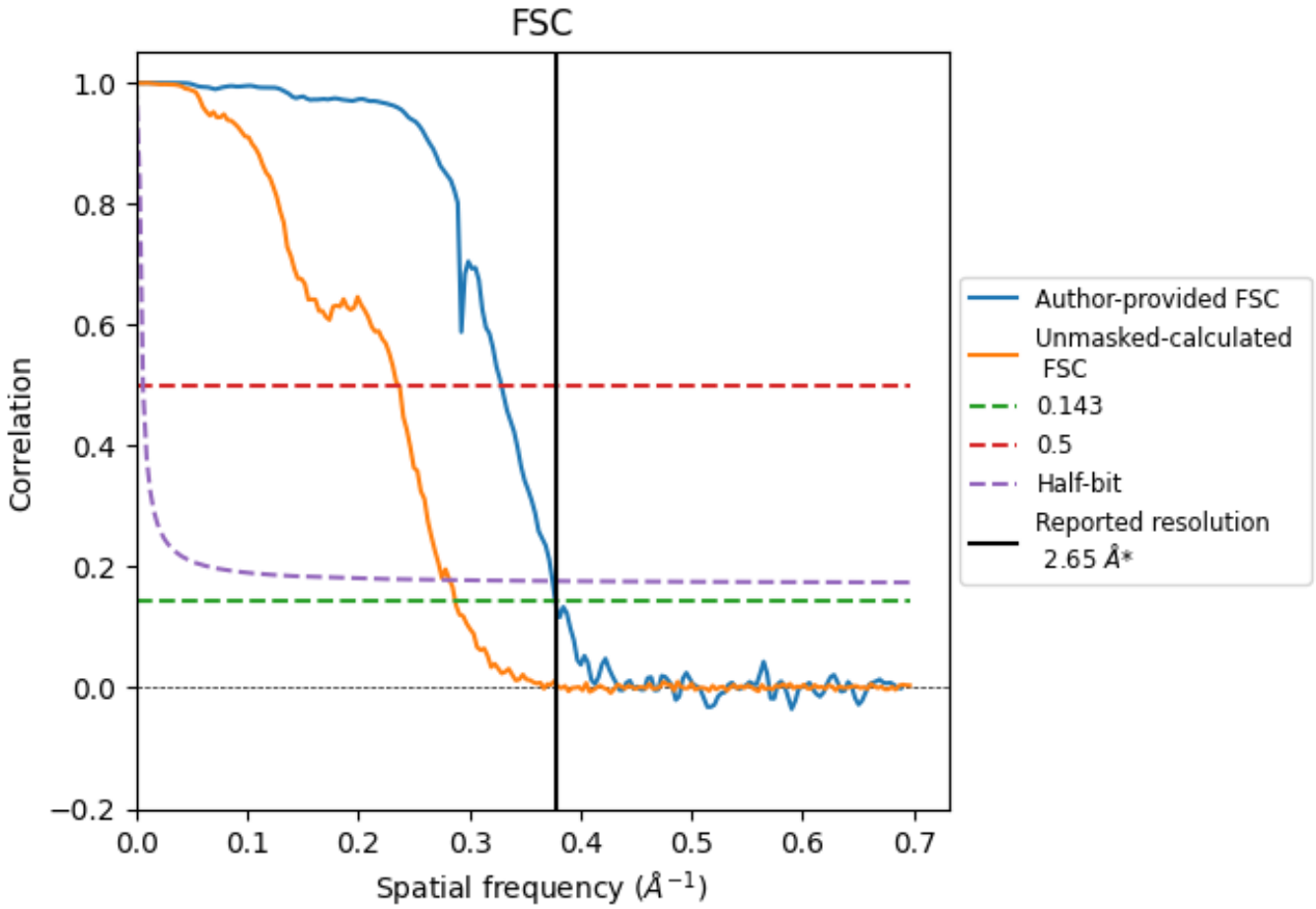


*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

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 0.377 Å^{-1}

8.2 Resolution estimates (i)

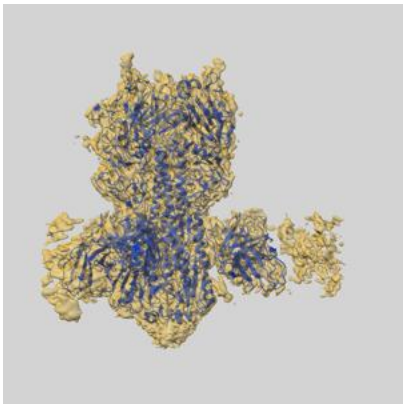
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.04	2.67
Unmasked-calculated*	3.48	4.23	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.65 by more than 10 %

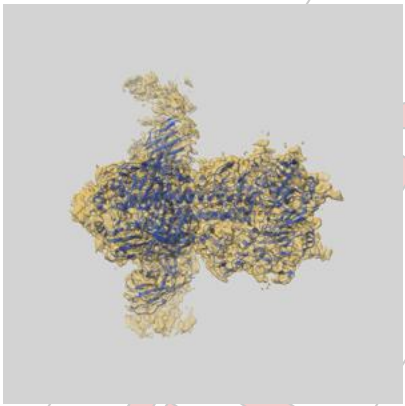
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70235 and PDB model 9O8S. Per-residue inclusion information can be found in section 3 on page 13.

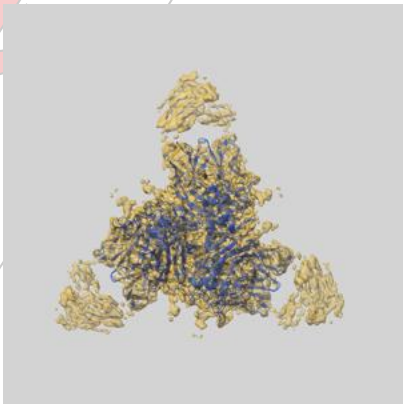
9.1 Map-model overlay



X



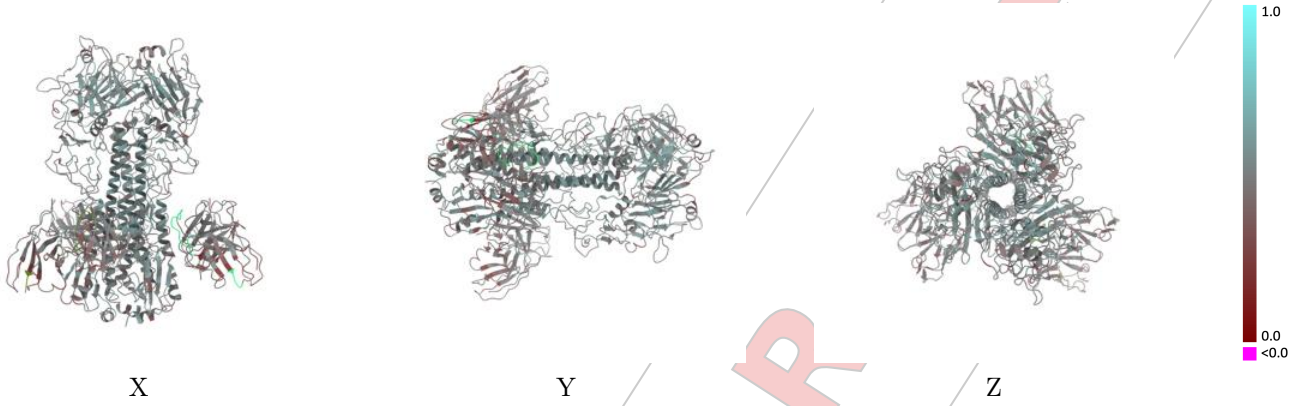
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

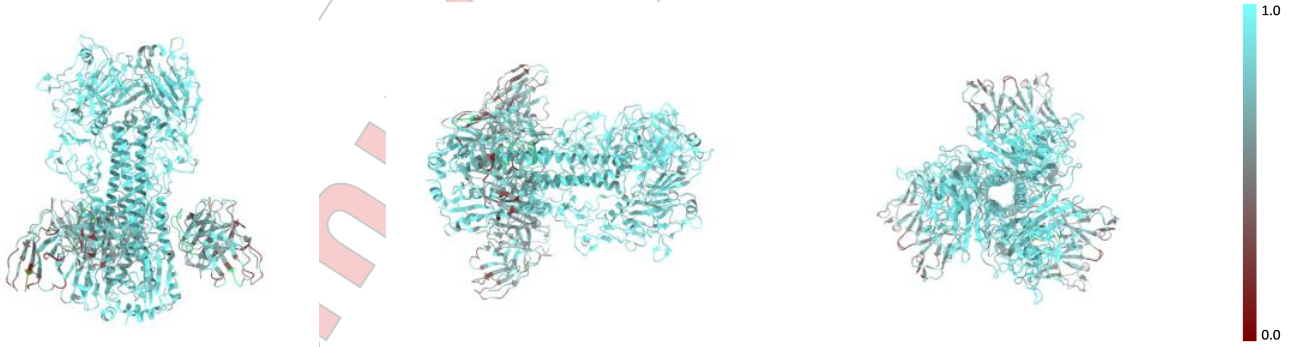
9.2 Q-score mapped to coordinate model



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.

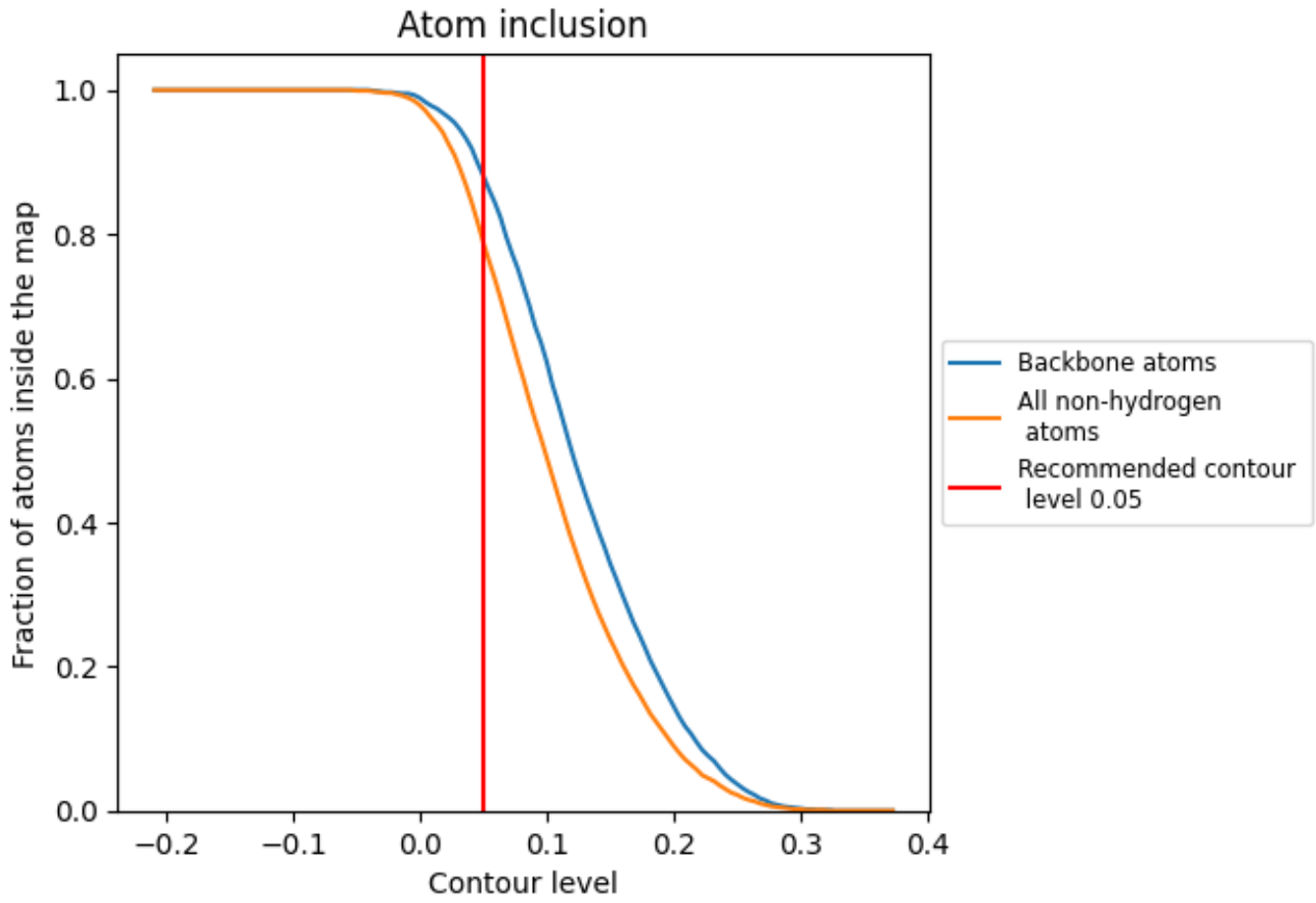
9.3 Atom inclusion mapped to coordinate model



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.4810
A	0.8550	0.5020
B	0.8750	0.5150
C	0.8560	0.4990
D	0.8550	0.5010
E	0.8720	0.5130
F	0.8760	0.5130
G	0.6380	0.4320
H	0.6320	0.4300
I	0.6320	0.4280
J	0.6230	0.4290
K	0.6260	0.4310
L	0.6250	0.4330
M	0.5000	0.4560
N	0.6050	0.4100
O	0.8570	0.5020
P	0.7690	0.4920
Q	0.6410	0.3300
R	0.5000	0.4480
S	0.6050	0.4220
T	0.8570	0.5060
U	0.7690	0.4950
V	0.5900	0.3050
W	0.5000	0.4640
X	0.6050	0.4120
Y	0.8570	0.5010
Z	0.7690	0.4870
a	0.6150	0.3440

Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 01:17 PM EDT

PDB ID	:	9O8T / pdb_00009o8t
EMDB ID	:	EMD-70236
Title	:	Cryo-EM structure of NI04359_d30_240 Fab in complex with influenza virus hemagglutinin from A/Michigan/45/2015 (H1N1)
Deposited on	:	2025-04-16
Resolution	:	3.12 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 ①) were used in the production of this report:

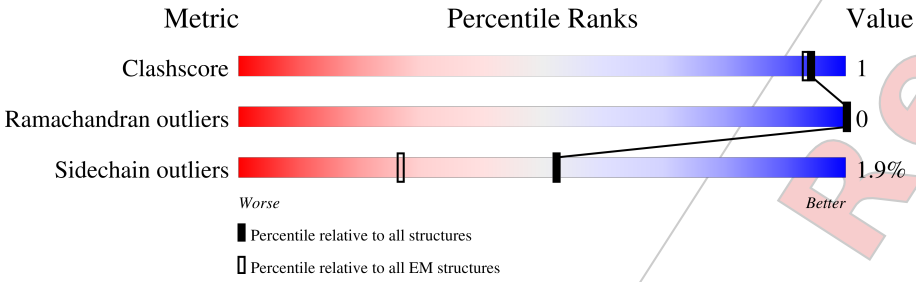
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.12 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	344	89% 5% 6%
1	C	344	88% 5% 6%
1	D	344	89% 5% 6%
2	B	233	70% 28%
2	E	233	70% 28%
2	F	233	70% 28%
3	G	130	22% 91% 6%

Continued on next page...

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Mol	Chain	Length	Quality of chain
3	H	130	24% 91% 6%
3	I	130	23% 91% 6%
4	J	107	21% 94%
4	K	107	21% 94%
4	L	107	21% 94%
5	M	2	50% 100%
5	N	2	50% 100%
5	O	2	50% 100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17142 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	C	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	D	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	167	Total	C	N	O	S	0	0
			1355	849	232	268	6		
2	E	167	Total	C	N	O	S	0	0
			1355	849	232	268	6		
2	F	167	Total	C	N	O	S	0	0
			1355	849	232	268	6		

There are 177 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	GLY	-	expression tag	UNP A0A1J0CXU0
B	176	GLY	-	expression tag	UNP A0A1J0CXU0
B	177	TYR	-	expression tag	UNP A0A1J0CXU0
B	178	ILE	-	expression tag	UNP A0A1J0CXU0
B	179	PRO	-	expression tag	UNP A0A1J0CXU0
B	180	GLU	-	expression tag	UNP A0A1J0CXU0
B	181	ALA	-	expression tag	UNP A0A1J0CXU0
B	182	PRO	-	expression tag	UNP A0A1J0CXU0
B	183	ARG	-	expression tag	UNP A0A1J0CXU0
B	184	ASP	-	expression tag	UNP A0A1J0CXU0
B	185	GLY	-	expression tag	UNP A0A1J0CXU0
B	186	GLN	-	expression tag	UNP A0A1J0CXU0
B	187	ALA	-	expression tag	UNP A0A1J0CXU0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	TYR	-	expression tag	UNP A0A1J0CXU0
B	189	VAL	-	expression tag	UNP A0A1J0CXU0
B	190	ARG	-	expression tag	UNP A0A1J0CXU0
B	191	LYS	-	expression tag	UNP A0A1J0CXU0
B	192	ASP	-	expression tag	UNP A0A1J0CXU0
B	193	GLY	-	expression tag	UNP A0A1J0CXU0
B	194	GLU	-	expression tag	UNP A0A1J0CXU0
B	195	TRP	-	expression tag	UNP A0A1J0CXU0
B	196	VAL	-	expression tag	UNP A0A1J0CXU0
B	197	LEU	-	expression tag	UNP A0A1J0CXU0
B	198	LEU	-	expression tag	UNP A0A1J0CXU0
B	199	SER	-	expression tag	UNP A0A1J0CXU0
B	200	THR	-	expression tag	UNP A0A1J0CXU0
B	201	PHE	-	expression tag	UNP A0A1J0CXU0
B	202	LEU	-	expression tag	UNP A0A1J0CXU0
B	203	GLY	-	expression tag	UNP A0A1J0CXU0
B	204	SER	-	expression tag	UNP A0A1J0CXU0
B	205	GLU	-	expression tag	UNP A0A1J0CXU0
B	206	ASN	-	expression tag	UNP A0A1J0CXU0
B	207	LEU	-	expression tag	UNP A0A1J0CXU0
B	208	TYR	-	expression tag	UNP A0A1J0CXU0
B	209	PHE	-	expression tag	UNP A0A1J0CXU0
B	210	GLN	-	expression tag	UNP A0A1J0CXU0
B	211	GLY	-	expression tag	UNP A0A1J0CXU0
B	212	SER	-	expression tag	UNP A0A1J0CXU0
B	213	HIS	-	expression tag	UNP A0A1J0CXU0
B	214	HIS	-	expression tag	UNP A0A1J0CXU0
B	215	HIS	-	expression tag	UNP A0A1J0CXU0
B	216	HIS	-	expression tag	UNP A0A1J0CXU0
B	217	HIS	-	expression tag	UNP A0A1J0CXU0
B	218	HIS	-	expression tag	UNP A0A1J0CXU0
B	219	GLY	-	expression tag	UNP A0A1J0CXU0
B	220	LEU	-	expression tag	UNP A0A1J0CXU0
B	221	ASN	-	expression tag	UNP A0A1J0CXU0
B	222	ASP	-	expression tag	UNP A0A1J0CXU0
B	223	ILE	-	expression tag	UNP A0A1J0CXU0
B	224	PHE	-	expression tag	UNP A0A1J0CXU0
B	225	GLU	-	expression tag	UNP A0A1J0CXU0
B	226	ALA	-	expression tag	UNP A0A1J0CXU0
B	227	GLN	-	expression tag	UNP A0A1J0CXU0
B	228	LYS	-	expression tag	UNP A0A1J0CXU0
B	229	ILE	-	expression tag	UNP A0A1J0CXU0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	230	GLU	-	expression tag	UNP A0A1J0CXU0
B	231	TRP	-	expression tag	UNP A0A1J0CXU0
B	232	HIS	-	expression tag	UNP A0A1J0CXU0
B	233	GLU	-	expression tag	UNP A0A1J0CXU0
E	175	GLY	-	expression tag	UNP A0A1J0CXU0
E	176	GLY	-	expression tag	UNP A0A1J0CXU0
E	177	TYR	-	expression tag	UNP A0A1J0CXU0
E	178	ILE	-	expression tag	UNP A0A1J0CXU0
E	179	PRO	-	expression tag	UNP A0A1J0CXU0
E	180	GLU	-	expression tag	UNP A0A1J0CXU0
E	181	ALA	-	expression tag	UNP A0A1J0CXU0
E	182	PRO	-	expression tag	UNP A0A1J0CXU0
E	183	ARG	-	expression tag	UNP A0A1J0CXU0
E	184	ASP	-	expression tag	UNP A0A1J0CXU0
E	185	GLY	-	expression tag	UNP A0A1J0CXU0
E	186	GLN	-	expression tag	UNP A0A1J0CXU0
E	187	ALA	-	expression tag	UNP A0A1J0CXU0
E	188	TYR	-	expression tag	UNP A0A1J0CXU0
E	189	VAL	-	expression tag	UNP A0A1J0CXU0
E	190	ARG	-	expression tag	UNP A0A1J0CXU0
E	191	LYS	-	expression tag	UNP A0A1J0CXU0
E	192	ASP	-	expression tag	UNP A0A1J0CXU0
E	193	GLY	-	expression tag	UNP A0A1J0CXU0
E	194	GLU	-	expression tag	UNP A0A1J0CXU0
E	195	TRP	-	expression tag	UNP A0A1J0CXU0
E	196	VAL	-	expression tag	UNP A0A1J0CXU0
E	197	LEU	-	expression tag	UNP A0A1J0CXU0
E	198	LEU	-	expression tag	UNP A0A1J0CXU0
E	199	SER	-	expression tag	UNP A0A1J0CXU0
E	200	THR	-	expression tag	UNP A0A1J0CXU0
E	201	PHE	-	expression tag	UNP A0A1J0CXU0
E	202	LEU	-	expression tag	UNP A0A1J0CXU0
E	203	GLY	-	expression tag	UNP A0A1J0CXU0
E	204	SER	-	expression tag	UNP A0A1J0CXU0
E	205	GLU	-	expression tag	UNP A0A1J0CXU0
E	206	ASN	-	expression tag	UNP A0A1J0CXU0
E	207	LEU	-	expression tag	UNP A0A1J0CXU0
E	208	TYR	-	expression tag	UNP A0A1J0CXU0
E	209	PHE	-	expression tag	UNP A0A1J0CXU0
E	210	GLN	-	expression tag	UNP A0A1J0CXU0
E	211	GLY	-	expression tag	UNP A0A1J0CXU0
E	212	SER	-	expression tag	UNP A0A1J0CXU0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	213	HIS	-	expression tag	UNP A0A1J0CXU0
E	214	HIS	-	expression tag	UNP A0A1J0CXU0
E	215	HIS	-	expression tag	UNP A0A1J0CXU0
E	216	HIS	-	expression tag	UNP A0A1J0CXU0
E	217	HIS	-	expression tag	UNP A0A1J0CXU0
E	218	HIS	-	expression tag	UNP A0A1J0CXU0
E	219	GLY	-	expression tag	UNP A0A1J0CXU0
E	220	LEU	-	expression tag	UNP A0A1J0CXU0
E	221	ASN	-	expression tag	UNP A0A1J0CXU0
E	222	ASP	-	expression tag	UNP A0A1J0CXU0
E	223	ILE	-	expression tag	UNP A0A1J0CXU0
E	224	PHE	-	expression tag	UNP A0A1J0CXU0
E	225	GLU	-	expression tag	UNP A0A1J0CXU0
E	226	ALA	-	expression tag	UNP A0A1J0CXU0
E	227	GLN	-	expression tag	UNP A0A1J0CXU0
E	228	LYS	-	expression tag	UNP A0A1J0CXU0
E	229	ILE	-	expression tag	UNP A0A1J0CXU0
E	230	GLU	-	expression tag	UNP A0A1J0CXU0
E	231	TRP	-	expression tag	UNP A0A1J0CXU0
E	232	HIS	-	expression tag	UNP A0A1J0CXU0
E	233	GLU	-	expression tag	UNP A0A1J0CXU0
F	175	GLY	-	expression tag	UNP A0A1J0CXU0
F	176	GLY	-	expression tag	UNP A0A1J0CXU0
F	177	TYR	-	expression tag	UNP A0A1J0CXU0
F	178	ILE	-	expression tag	UNP A0A1J0CXU0
F	179	PRO	-	expression tag	UNP A0A1J0CXU0
F	180	GLU	-	expression tag	UNP A0A1J0CXU0
F	181	ALA	-	expression tag	UNP A0A1J0CXU0
F	182	PRO	-	expression tag	UNP A0A1J0CXU0
F	183	ARG	-	expression tag	UNP A0A1J0CXU0
F	184	ASP	-	expression tag	UNP A0A1J0CXU0
F	185	GLY	-	expression tag	UNP A0A1J0CXU0
F	186	GLN	-	expression tag	UNP A0A1J0CXU0
F	187	ALA	-	expression tag	UNP A0A1J0CXU0
F	188	TYR	-	expression tag	UNP A0A1J0CXU0
F	189	VAL	-	expression tag	UNP A0A1J0CXU0
F	190	ARG	-	expression tag	UNP A0A1J0CXU0
F	191	LYS	-	expression tag	UNP A0A1J0CXU0
F	192	ASP	-	expression tag	UNP A0A1J0CXU0
F	193	GLY	-	expression tag	UNP A0A1J0CXU0
F	194	GLU	-	expression tag	UNP A0A1J0CXU0
F	195	TRP	-	expression tag	UNP A0A1J0CXU0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	196	VAL	-	expression tag	UNP A0A1J0CXU0
F	197	LEU	-	expression tag	UNP A0A1J0CXU0
F	198	LEU	-	expression tag	UNP A0A1J0CXU0
F	199	SER	-	expression tag	UNP A0A1J0CXU0
F	200	THR	-	expression tag	UNP A0A1J0CXU0
F	201	PHE	-	expression tag	UNP A0A1J0CXU0
F	202	LEU	-	expression tag	UNP A0A1J0CXU0
F	203	GLY	-	expression tag	UNP A0A1J0CXU0
F	204	SER	-	expression tag	UNP A0A1J0CXU0
F	205	GLU	-	expression tag	UNP A0A1J0CXU0
F	206	ASN	-	expression tag	UNP A0A1J0CXU0
F	207	LEU	-	expression tag	UNP A0A1J0CXU0
F	208	TYR	-	expression tag	UNP A0A1J0CXU0
F	209	PHE	-	expression tag	UNP A0A1J0CXU0
F	210	GLN	-	expression tag	UNP A0A1J0CXU0
F	211	GLY	-	expression tag	UNP A0A1J0CXU0
F	212	SER	-	expression tag	UNP A0A1J0CXU0
F	213	HIS	-	expression tag	UNP A0A1J0CXU0
F	214	HIS	-	expression tag	UNP A0A1J0CXU0
F	215	HIS	-	expression tag	UNP A0A1J0CXU0
F	216	HIS	-	expression tag	UNP A0A1J0CXU0
F	217	HIS	-	expression tag	UNP A0A1J0CXU0
F	218	HIS	-	expression tag	UNP A0A1J0CXU0
F	219	GLY	-	expression tag	UNP A0A1J0CXU0
F	220	LEU	-	expression tag	UNP A0A1J0CXU0
F	221	ASN	-	expression tag	UNP A0A1J0CXU0
F	222	ASP	-	expression tag	UNP A0A1J0CXU0
F	223	ILE	-	expression tag	UNP A0A1J0CXU0
F	224	PHE	-	expression tag	UNP A0A1J0CXU0
F	225	GLU	-	expression tag	UNP A0A1J0CXU0
F	226	ALA	-	expression tag	UNP A0A1J0CXU0
F	227	GLN	-	expression tag	UNP A0A1J0CXU0
F	228	LYS	-	expression tag	UNP A0A1J0CXU0
F	229	ILE	-	expression tag	UNP A0A1J0CXU0
F	230	GLU	-	expression tag	UNP A0A1J0CXU0
F	231	TRP	-	expression tag	UNP A0A1J0CXU0
F	232	HIS	-	expression tag	UNP A0A1J0CXU0
F	233	GLU	-	expression tag	UNP A0A1J0CXU0

- Molecule 3 is a protein called NI04359_d30_240 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	128	Total	C	N	O	S	0	0
			971	608	167	189	7		
3	G	128	Total	C	N	O	S	0	0
			971	608	167	189	7		
3	I	128	Total	C	N	O	S	0	0
			971	608	167	189	7		

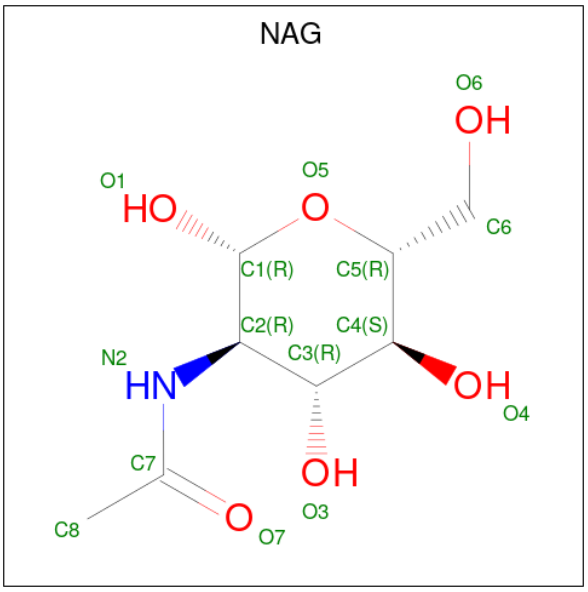
- Molecule 4 is a protein called NI04359_d30_240 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	105	Total	C	N	O	S	0	0
			790	492	129	166	3		
4	J	105	Total	C	N	O	S	0	0
			790	492	129	166	3		
4	K	105	Total	C	N	O	S	0	0
			790	492	129	166	3		

- Molecule 5 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
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	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



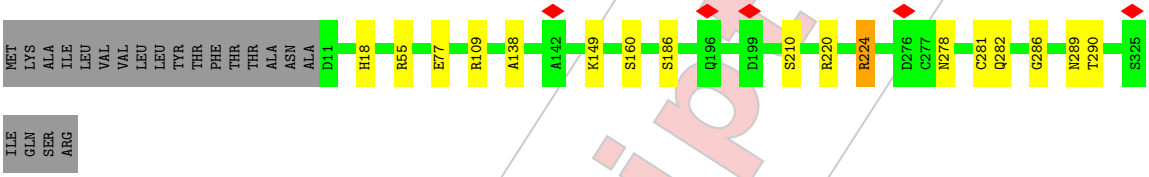
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	C	1	14	8	1	5	0
6	C	1	14	8	1	5	0
6	E	1	14	8	1	5	0
6	D	1	14	8	1	5	0
6	D	1	14	8	1	5	0
6	F	1	14	8	1	5	0

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.

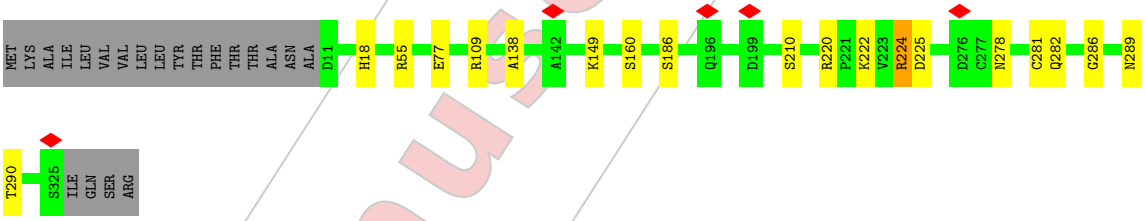
- Molecule 1: Hemagglutinin HA1

Chain A:



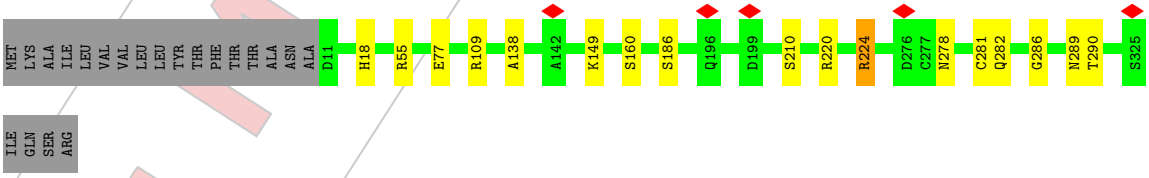
- Molecule 1: Hemagglutinin HA1

Chain C:



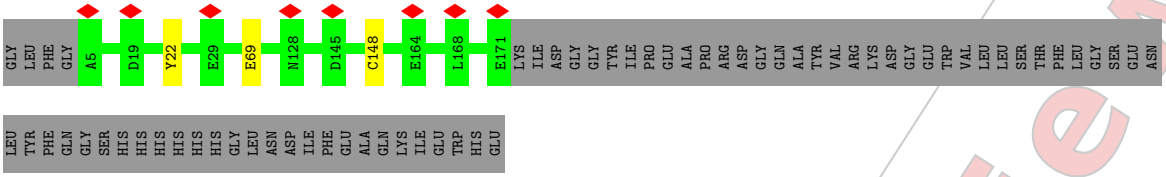
- Molecule 1: Hemagglutinin HA1

Chain D:



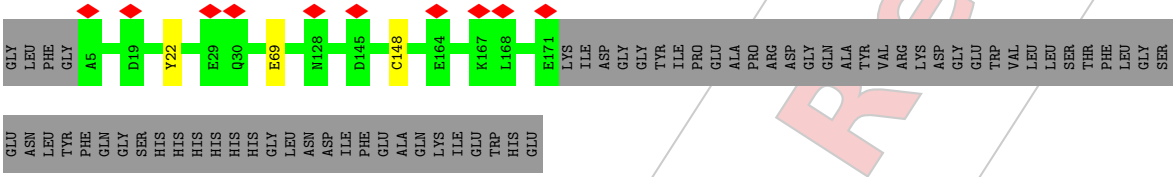
- Molecule 2: Hemagglutinin HA2

Chain B:



• Molecule 2: Hemagglutinin HA2

Chain E:

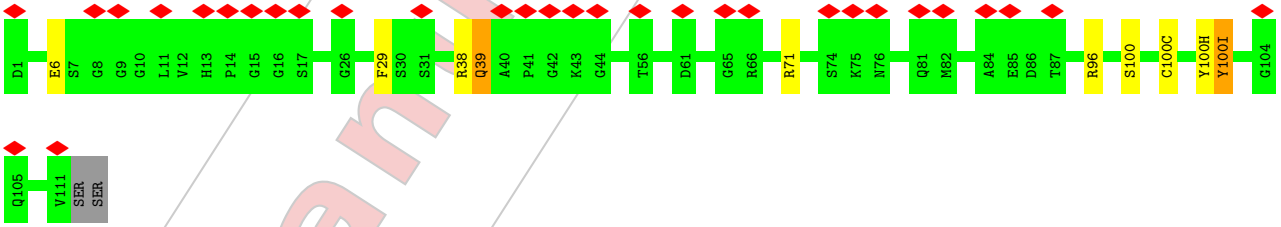


• Molecule 2: Hemagglutinin HA2

Chain F:

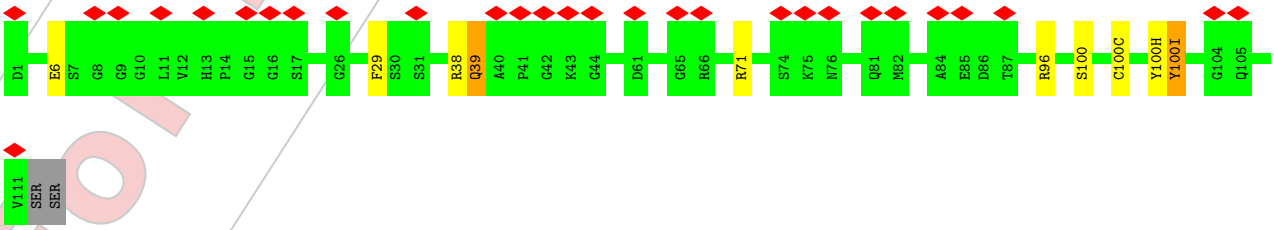
• Molecule 3: NI04359_d30_240 Fab heavy chain

Chain H:



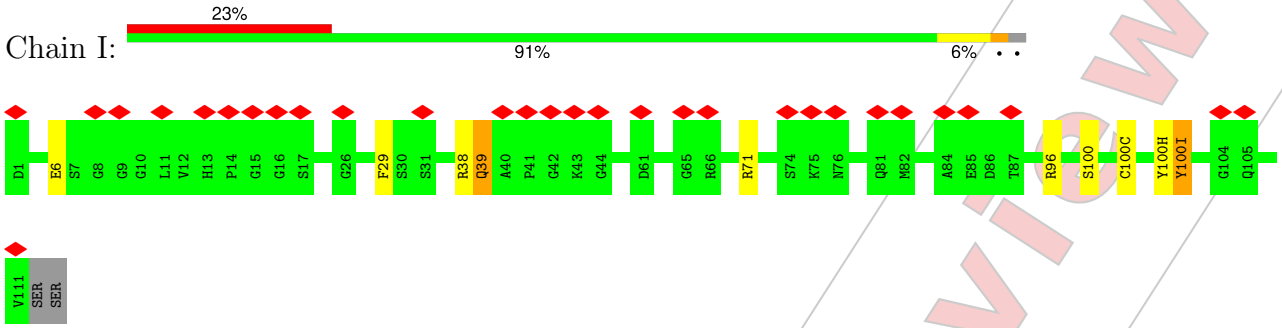
• Molecule 3: NI04359_d30_240 Fab heavy chain

Chain G:



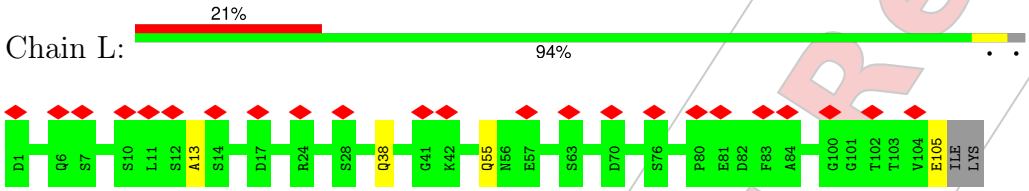
• Molecule 3: NI04359_d30_240 Fab heavy chain

Chain I:



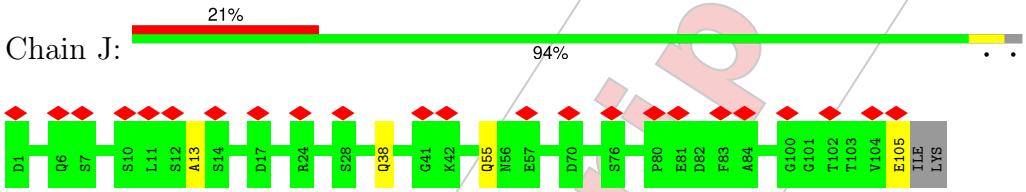
• Molecule 4: NI04359_d30_240 Fab light chain

Chain L:



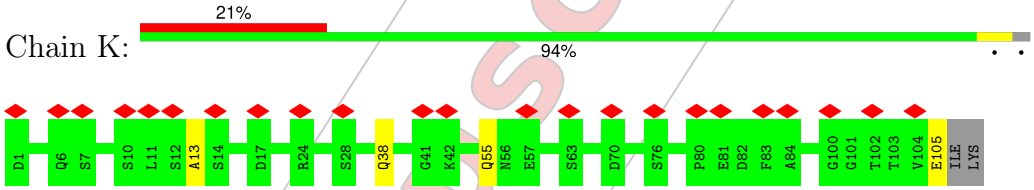
• Molecule 4: NI04359_d30_240 Fab light chain

Chain J:



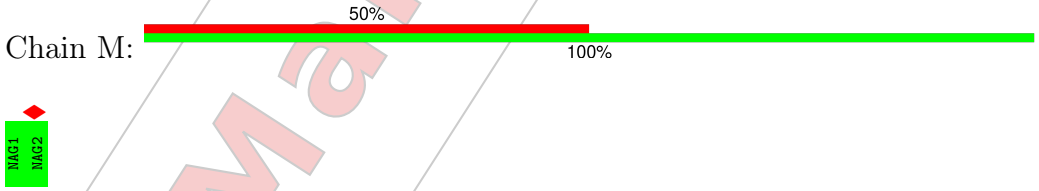
• Molecule 4: NI04359_d30_240 Fab light chain

Chain K:



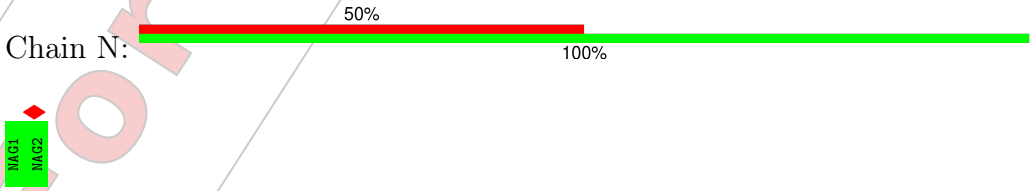
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



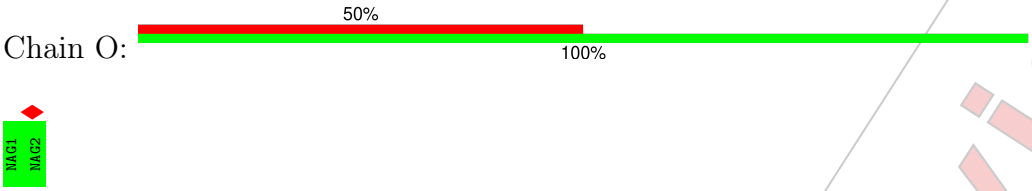
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	84345	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	44.87	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.869	Depositor
Minimum map value	-0.717	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	319.0, 319.0, 319.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/2591	0.60	0/3525
1	C	0.31	0/2591	0.60	0/3525
1	D	0.31	0/2591	0.60	0/3525
2	B	0.29	0/1382	0.54	0/1862
2	E	0.29	0/1382	0.54	0/1862
2	F	0.29	0/1382	0.54	0/1862
3	G	0.32	0/993	0.74	3/1343 (0.2%)
3	H	0.32	0/993	0.74	3/1343 (0.2%)
3	I	0.32	0/993	0.74	3/1343 (0.2%)
4	J	0.29	0/807	0.60	0/1097
4	K	0.29	0/807	0.59	0/1097
4	L	0.29	0/807	0.59	0/1097
All	All	0.30	0/17319	0.61	9/23481 (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
1	A	0	2
1	C	0	2
1	D	0	2
3	G	0	1
3	H	0	1
3	I	0	1
All	All	0	9

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	100(I)	TYR	CA-CB-CG	8.00	128.59	113.40
3	I	100(I)	TYR	CA-CB-CG	7.98	128.56	113.40
3	G	100(I)	TYR	CA-CB-CG	7.97	128.55	113.40
3	G	100(I)	TYR	CB-CG-CD1	7.61	125.57	121.00
3	I	100(I)	TYR	CB-CG-CD1	7.61	125.56	121.00
3	H	100(I)	TYR	CB-CG-CD1	7.60	125.56	121.00
3	I	100(I)	TYR	CB-CG-CD2	-5.40	117.76	121.00
3	G	100(I)	TYR	CB-CG-CD2	-5.38	117.77	121.00
3	H	100(I)	TYR	CB-CG-CD2	-5.32	117.81	121.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	55	ARG	Sidechain
1	C	224	ARG	Sidechain
1	C	55	ARG	Sidechain
1	D	224	ARG	Sidechain
1	D	55	ARG	Sidechain
3	G	38	ARG	Sidechain
3	H	38	ARG	Sidechain
3	I	38	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2461	6	0
1	C	2528	0	2461	7	0
1	D	2528	0	2461	6	0
2	B	1355	0	1281	1	0
2	E	1355	0	1281	1	0
2	F	1355	0	1281	1	0
3	G	971	0	919	5	0
3	H	971	0	919	5	0
3	I	971	0	919	5	0
4	J	790	0	756	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	790	0	756	3	0
4	L	790	0	756	3	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
6	C	28	0	26	0	0
6	D	28	0	26	0	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
All	All	17142	0	16443	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (37) 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:A:282:GLN:NE2	1:A:286:GLY:O	2.15	0.79
1:C:282:GLN:NE2	1:C:286:GLY:O	2.15	0.79
1:D:282:GLN:NE2	1:D:286:GLY:O	2.15	0.79
3:I:29:PHE:O	3:I:71:ARG:NH2	2.19	0.76
3:H:29:PHE:O	3:H:71:ARG:NH2	2.19	0.76
3:G:29:PHE:O	3:G:71:ARG:NH2	2.19	0.75
4:J:13:ALA:N	4:J:105:GLU:O	2.28	0.67
4:L:13:ALA:N	4:L:105:GLU:O	2.28	0.66
4:K:13:ALA:N	4:K:105:GLU:O	2.28	0.66
1:A:281:CYS:SG	1:A:282:GLN:N	2.74	0.61
1:D:281:CYS:SG	1:D:282:GLN:N	2.74	0.61
1:C:281:CYS:SG	1:C:282:GLN:N	2.74	0.60
1:C:109:ARG:NE	2:E:69:GLU:OE1	2.33	0.59
1:A:109:ARG:NE	2:B:69:GLU:OE1	2.33	0.58
1:D:109:ARG:NE	2:F:69:GLU:OE1	2.33	0.55
3:G:96:ARG:NH2	3:G:100:SER:O	2.45	0.50
3:H:96:ARG:NH2	3:H:100:SER:O	2.45	0.50
3:I:96:ARG:NH2	3:I:100:SER:O	2.45	0.48
1:C:138:ALA:O	1:C:224:ARG:NH2	2.46	0.48
1:A:138:ALA:O	1:A:224:ARG:NH2	2.47	0.47
1:D:138:ALA:O	1:D:224:ARG:NH2	2.47	0.47
3:I:96:ARG:NH1	4:K:55:GLN:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:96:ARG:NH1	4:J:55:GLN:OE1	2.49	0.46
3:H:96:ARG:NH1	4:L:55:GLN:OE1	2.48	0.46
1:A:289:ASN:O	1:A:290:THR:OG1	2.35	0.45
1:C:289:ASN:O	1:C:290:THR:OG1	2.35	0.45
1:D:289:ASN:O	1:D:290:THR:OG1	2.34	0.45
1:A:77:GLU:OE1	1:A:149:LYS:NZ	2.52	0.43
3:G:6:GLU:N	3:G:6:GLU:OE1	2.52	0.43
3:I:39:GLN:OE1	4:K:38:GLN:NE2	2.45	0.42
3:G:39:GLN:OE1	4:J:38:GLN:NE2	2.45	0.42
1:D:77:GLU:OE1	1:D:149:LYS:NZ	2.52	0.42
3:I:6:GLU:N	3:I:6:GLU:OE1	2.52	0.42
1:C:222:LYS:NZ	1:C:225:ASP:O	2.52	0.42
1:C:77:GLU:OE1	1:C:149:LYS:NZ	2.52	0.42
3:H:6:GLU:N	3:H:6:GLU:OE1	2.52	0.42
3:H:39:GLN:OE1	4:L:38:GLN:NE2	2.45	0.42

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	321/344 (93%)	306 (95%)	15 (5%)	0	100	100
1	C	321/344 (93%)	307 (96%)	14 (4%)	0	100	100
1	D	321/344 (93%)	306 (95%)	15 (5%)	0	100	100
2	B	165/233 (71%)	161 (98%)	4 (2%)	0	100	100
2	E	165/233 (71%)	161 (98%)	4 (2%)	0	100	100
2	F	165/233 (71%)	161 (98%)	4 (2%)	0	100	100
3	G	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
3	H	126/130 (97%)	123 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
4	J	103/107 (96%)	95 (92%)	8 (8%)	0	100	100
4	K	103/107 (96%)	95 (92%)	8 (8%)	0	100	100
4	L	103/107 (96%)	95 (92%)	8 (8%)	0	100	100
All	All	2145/2442 (88%)	2056 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/302 (94%)	278 (98%)	6 (2%)	48	71
1	C	284/302 (94%)	278 (98%)	6 (2%)	48	71
1	D	284/302 (94%)	278 (98%)	6 (2%)	48	71
2	B	145/199 (73%)	143 (99%)	2 (1%)	62	79
2	E	145/199 (73%)	143 (99%)	2 (1%)	62	79
2	F	145/199 (73%)	143 (99%)	2 (1%)	62	79
3	G	102/104 (98%)	98 (96%)	4 (4%)	27	56
3	H	102/104 (98%)	98 (96%)	4 (4%)	27	56
3	I	102/104 (98%)	98 (96%)	4 (4%)	27	56
4	J	91/93 (98%)	91 (100%)	0	100	100
4	K	91/93 (98%)	91 (100%)	0	100	100
4	L	91/93 (98%)	91 (100%)	0	100	100
All	All	1866/2094 (89%)	1830 (98%)	36 (2%)	52	73

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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Mol	Chain	Res	Type
1	A	160	SER
1	A	186	SER
1	A	210	SER
1	A	220	ARG
1	A	278	ASN
2	B	22	TYR
2	B	148	CYS
3	H	39	GLN
3	H	100(C)	CYS
3	H	100(H)	TYR
3	H	100(I)	TYR
1	C	18	HIS
1	C	160	SER
1	C	186	SER
1	C	210	SER
1	C	220	ARG
1	C	278	ASN
2	E	22	TYR
2	E	148	CYS
3	G	39	GLN
3	G	100(C)	CYS
3	G	100(H)	TYR
3	G	100(I)	TYR
1	D	18	HIS
1	D	160	SER
1	D	186	SER
1	D	210	SER
1	D	220	ARG
1	D	278	ASN
2	F	22	TYR
2	F	148	CYS
3	I	39	GLN
3	I	100(C)	CYS
3	I	100(H)	TYR
3	I	100(I)	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 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	1,5	14,14,15	0.25	0	17,19,21	0.53	0
5	NAG	M	2	5	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	N	1	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	N	2	5	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	O	1	1,5	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	O	2	5	14,14,15	0.22	0	17,19,21	0.44	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
5	NAG	M	1	1,5	-	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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

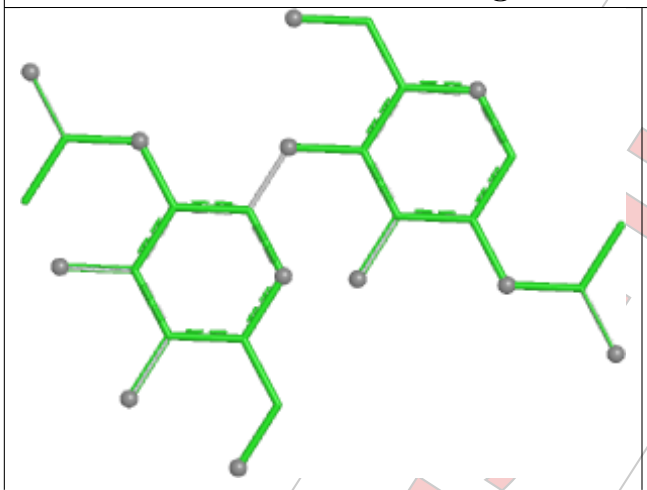
Mol	Chain	Res	Type	Atoms
5	O	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6

There are no ring outliers.

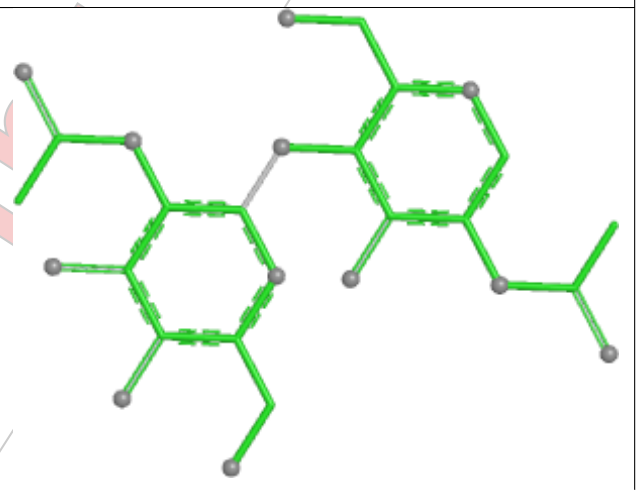
No monomer is involved in short contacts.

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

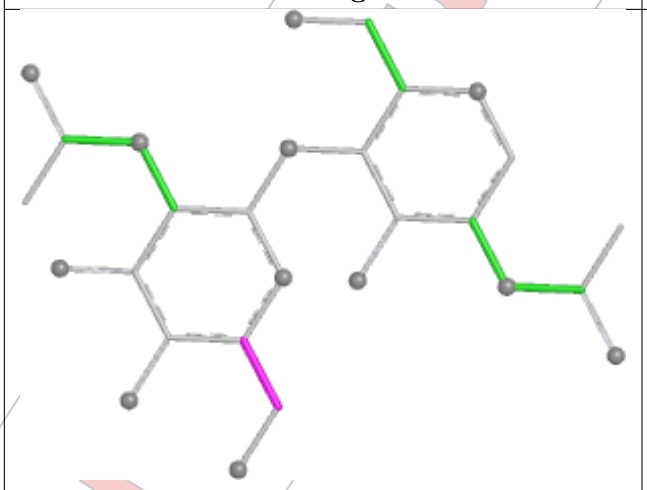
Oligosaccharide Chain M



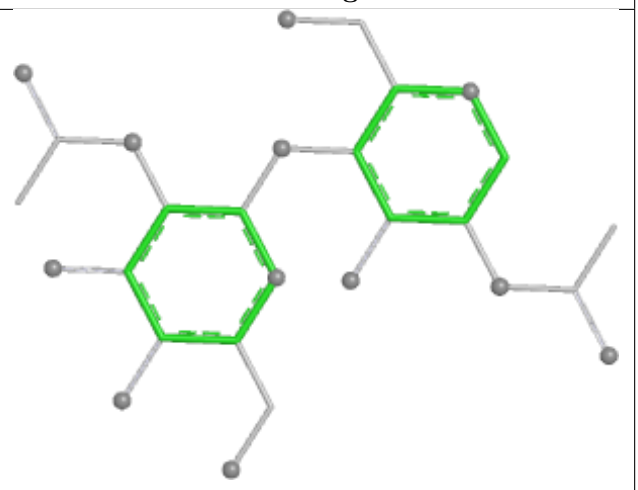
Bond lengths



Bond angles

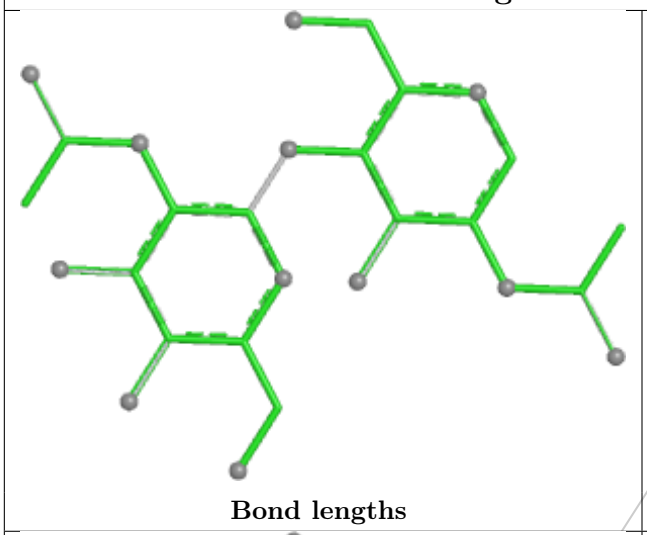


Torsions

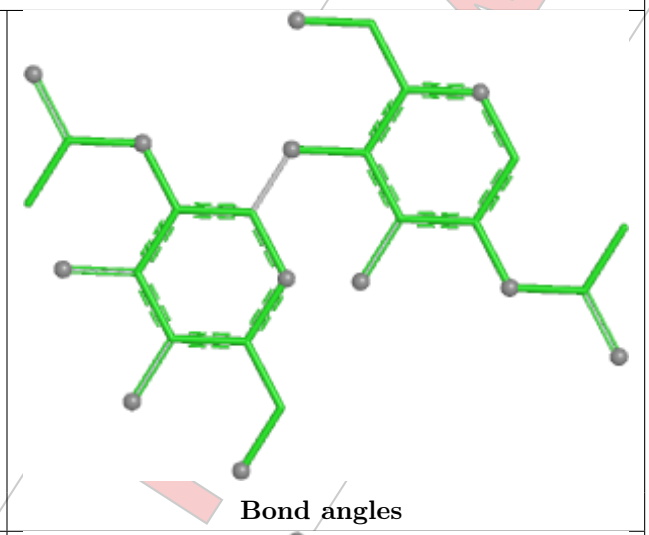


Rings

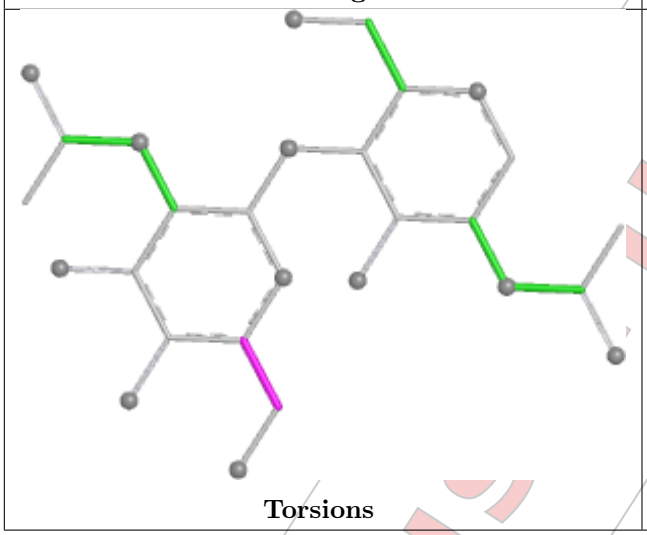
Oligosaccharide Chain N



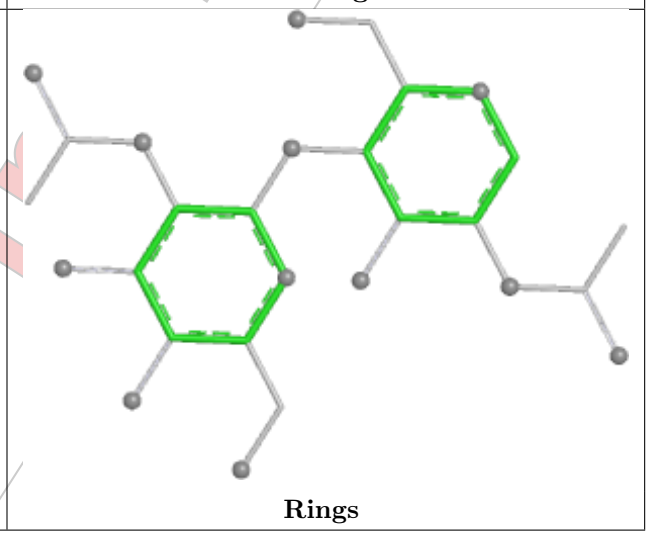
Bond lengths



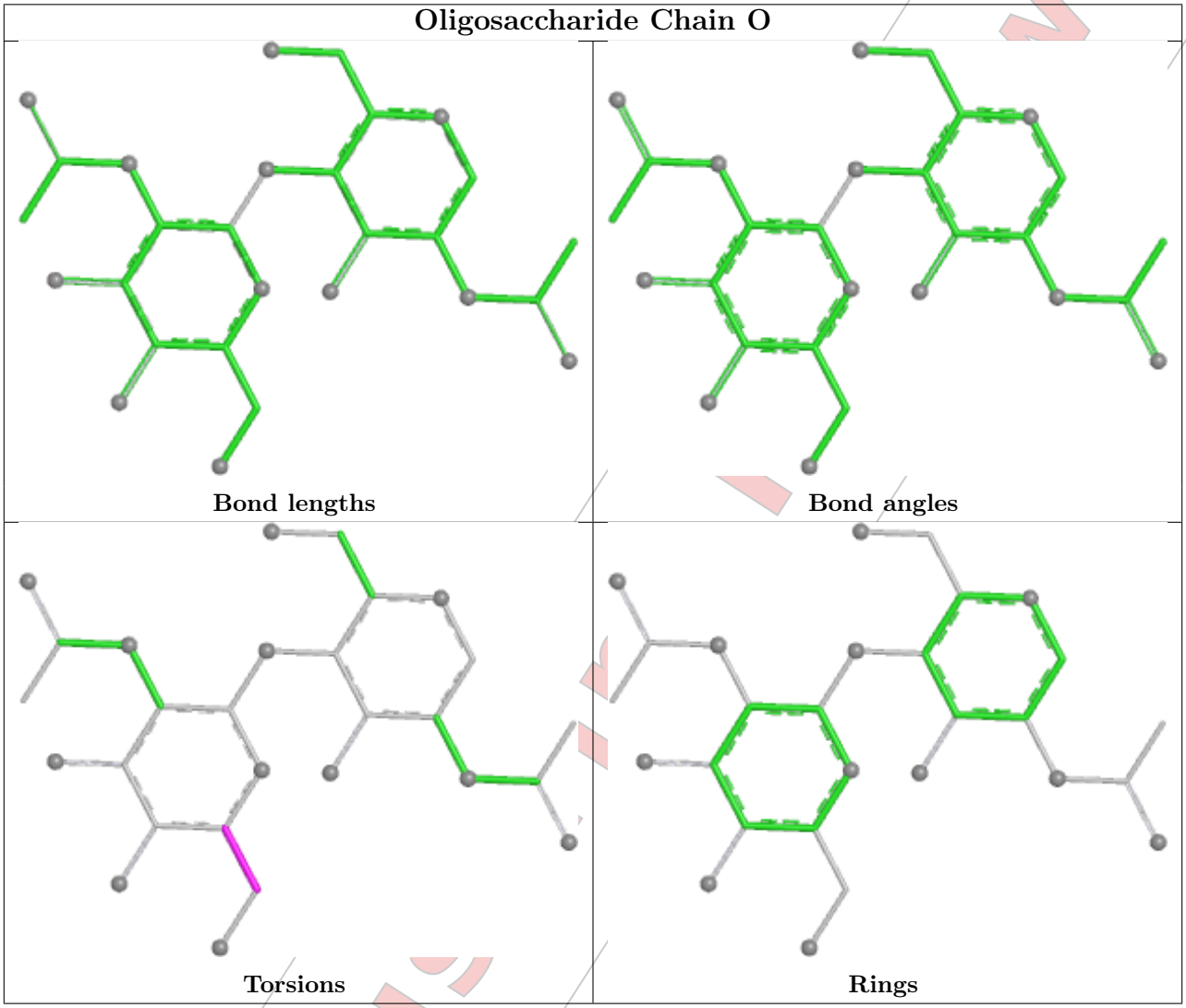
Bond angles



Torsions



Rings



5.6 Ligand geometry

9 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	$\#\|Z\|>2$
6	NAG	C	401	1	14,14,15	0.46	0	17,19,21	0.61	1 (5%)
6	NAG	D	401	1	14,14,15	0.45	0	17,19,21	0.61	1 (5%)
6	NAG	A	401	1	14,14,15	0.45	0	17,19,21	0.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	C	402	1	14,14,15	0.45	0	17,19,21	0.65	1 (5%)
6	NAG	B	301	2	14,14,15	0.32	0	17,19,21	0.55	0
6	NAG	A	402	1	14,14,15	0.47	0	17,19,21	0.66	1 (5%)
6	NAG	E	301	2	14,14,15	0.32	0	17,19,21	0.56	0
6	NAG	D	402	1	14,14,15	0.46	0	17,19,21	0.66	1 (5%)
6	NAG	F	301	2	14,14,15	0.32	0	17,19,21	0.56	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	C	401	1	-	2/6/23/26	0/1/1/1
6	NAG	D	401	1	-	1/6/23/26	0/1/1/1
6	NAG	A	401	1	-	1/6/23/26	0/1/1/1
6	NAG	C	402	1	-	0/6/23/26	0/1/1/1
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
6	NAG	A	402	1	-	0/6/23/26	0/1/1/1
6	NAG	E	301	2	-	0/6/23/26	0/1/1/1
6	NAG	D	402	1	-	0/6/23/26	0/1/1/1
6	NAG	F	301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	402	NAG	C1-O5-C5	2.41	115.42	112.19
6	A	402	NAG	C1-O5-C5	2.40	115.40	112.19
6	C	402	NAG	C1-O5-C5	2.39	115.39	112.19
6	C	401	NAG	C1-O5-C5	2.11	115.01	112.19
6	D	401	NAG	C1-O5-C5	2.07	114.96	112.19
6	A	401	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	C4-C5-C6-O6
6	C	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	D	401	NAG	C4-C5-C6-O6
6	C	401	NAG	C1-C2-N2-C7

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.

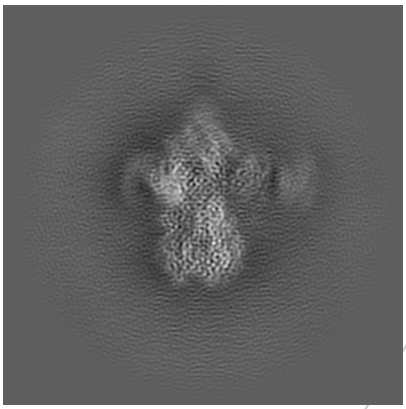
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70236. These allow visual inspection of the internal detail of the map and identification of artifacts.

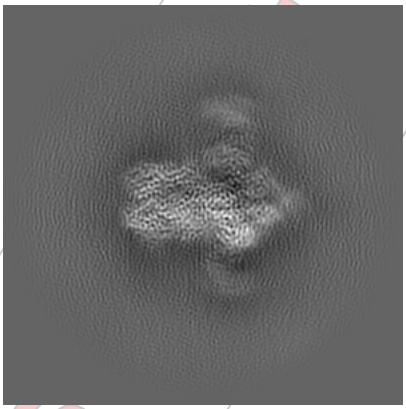
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

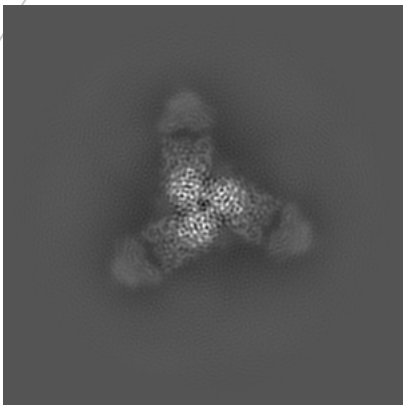
6.1.1 Primary map



X

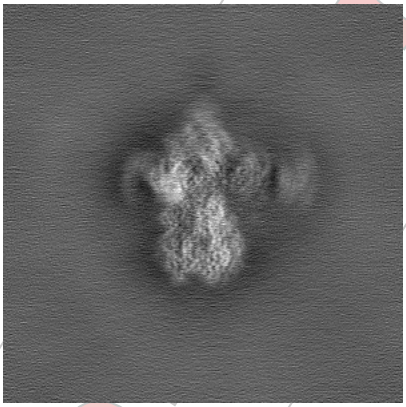


Y

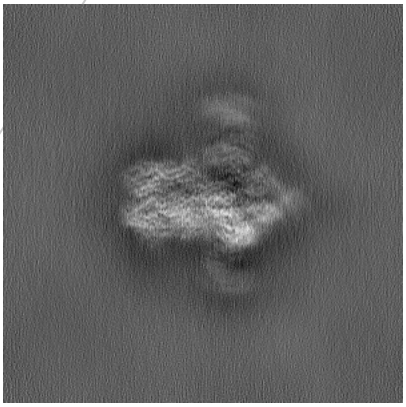


Z

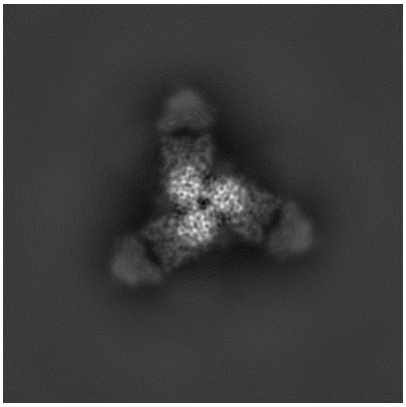
6.1.2 Raw map



X



Y

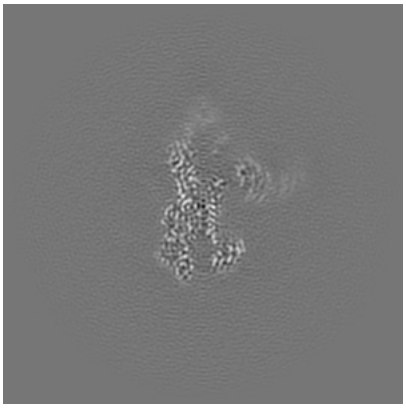


Z

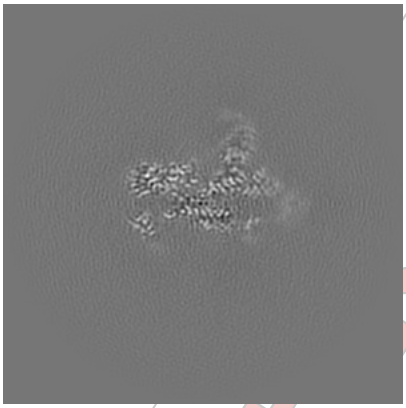
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

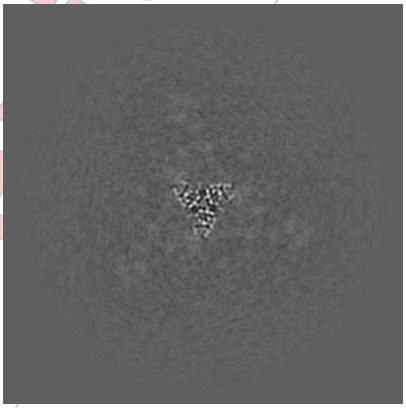
6.2.1 Primary map



X Index: 220

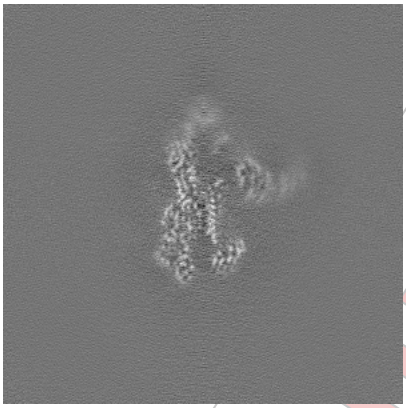


Y Index: 220

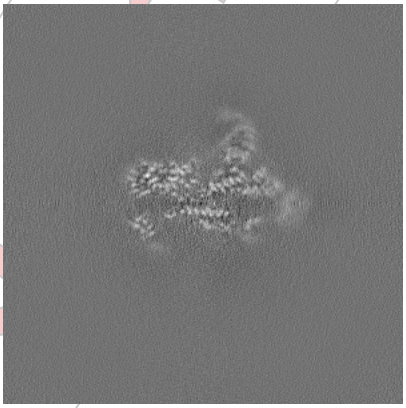


Z Index: 220

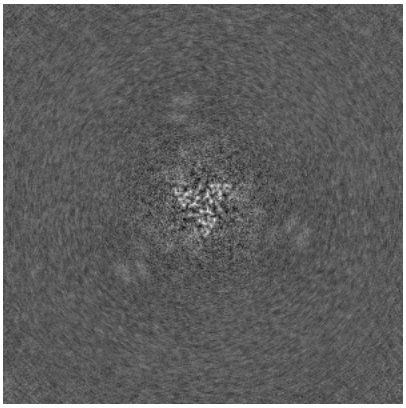
6.2.2 Raw map



X Index: 220



Y Index: 220

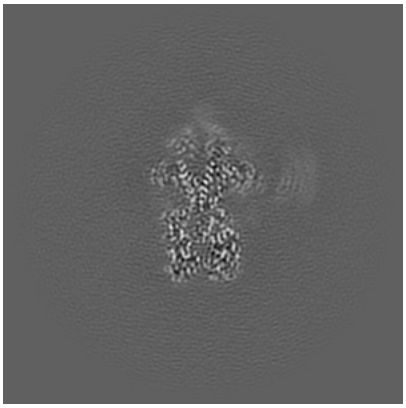


Z Index: 220

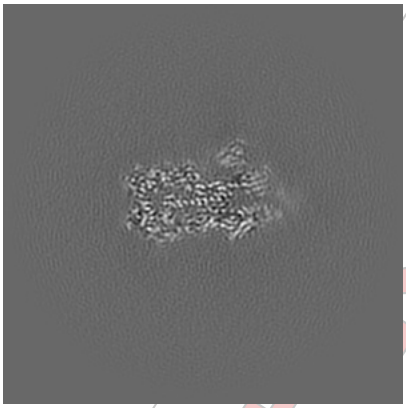
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

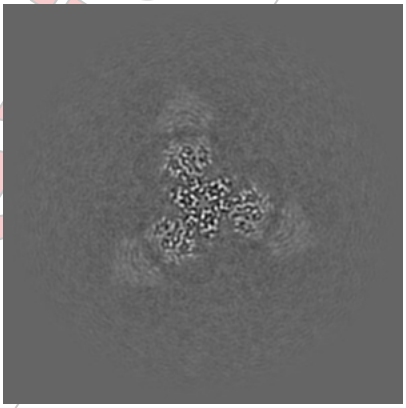
6.3.1 Primary map



X Index: 207

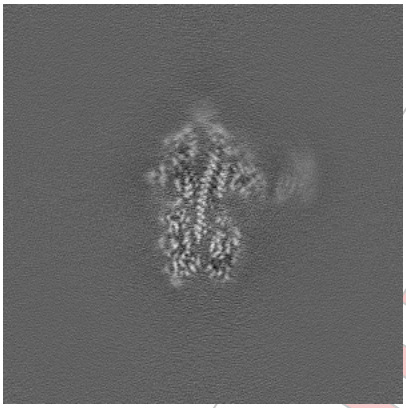


Y Index: 232

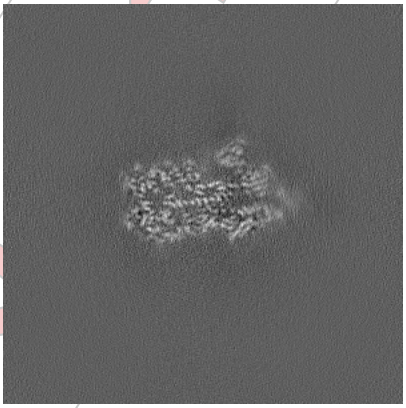


Z Index: 247

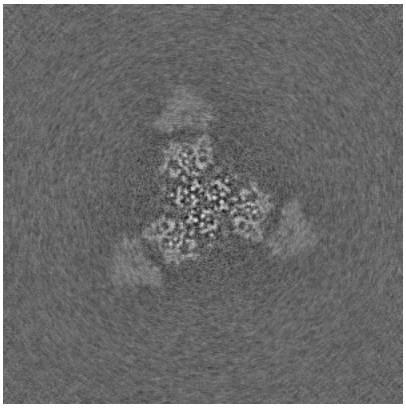
6.3.2 Raw map



X Index: 210



Y Index: 232

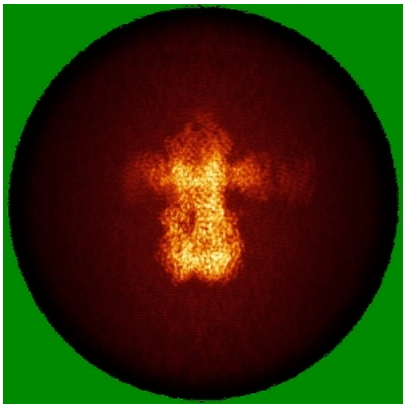


Z Index: 247

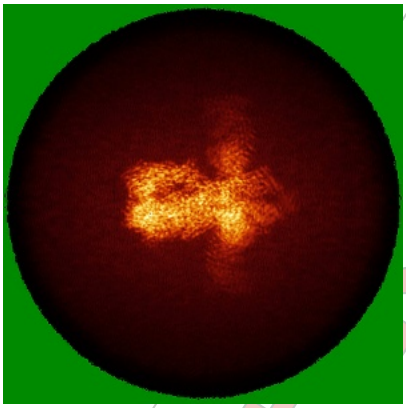
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

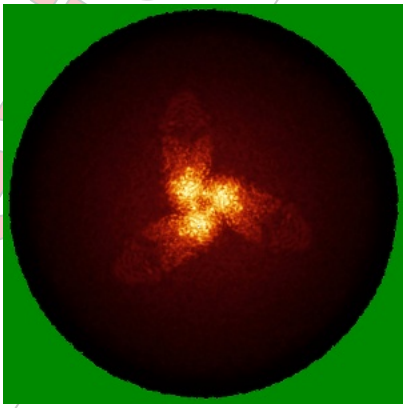
6.4.1 Primary map



X

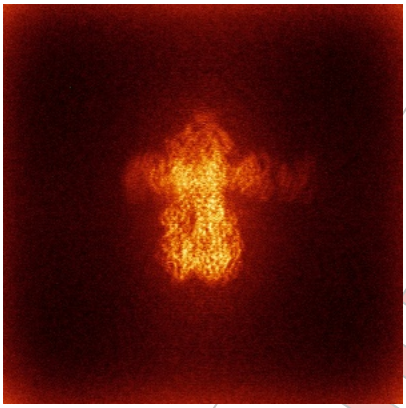


Y

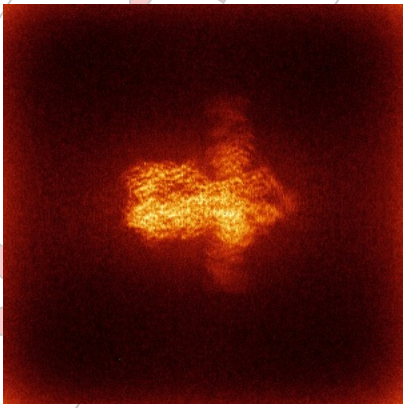


Z

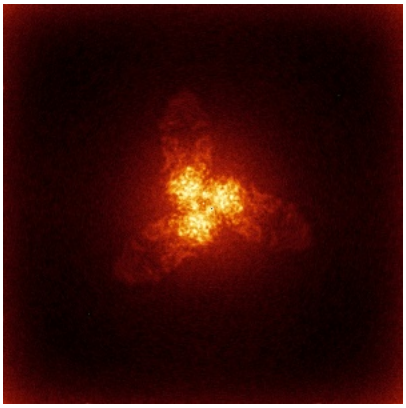
6.4.2 Raw map



X



Y

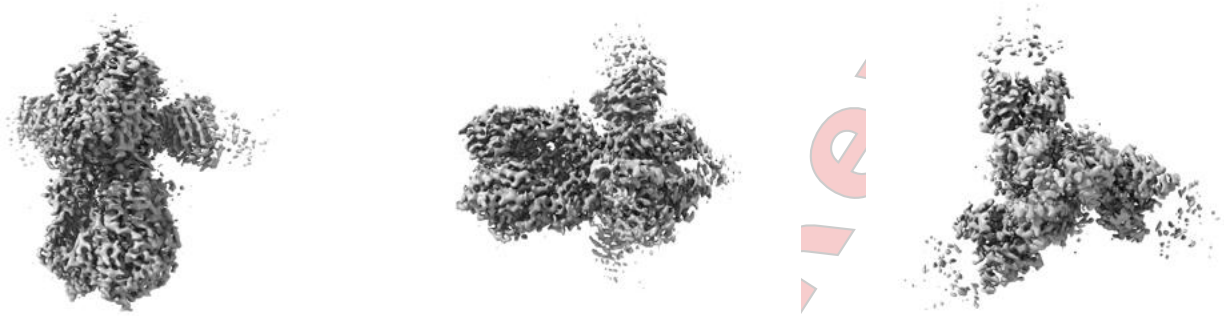


Z

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

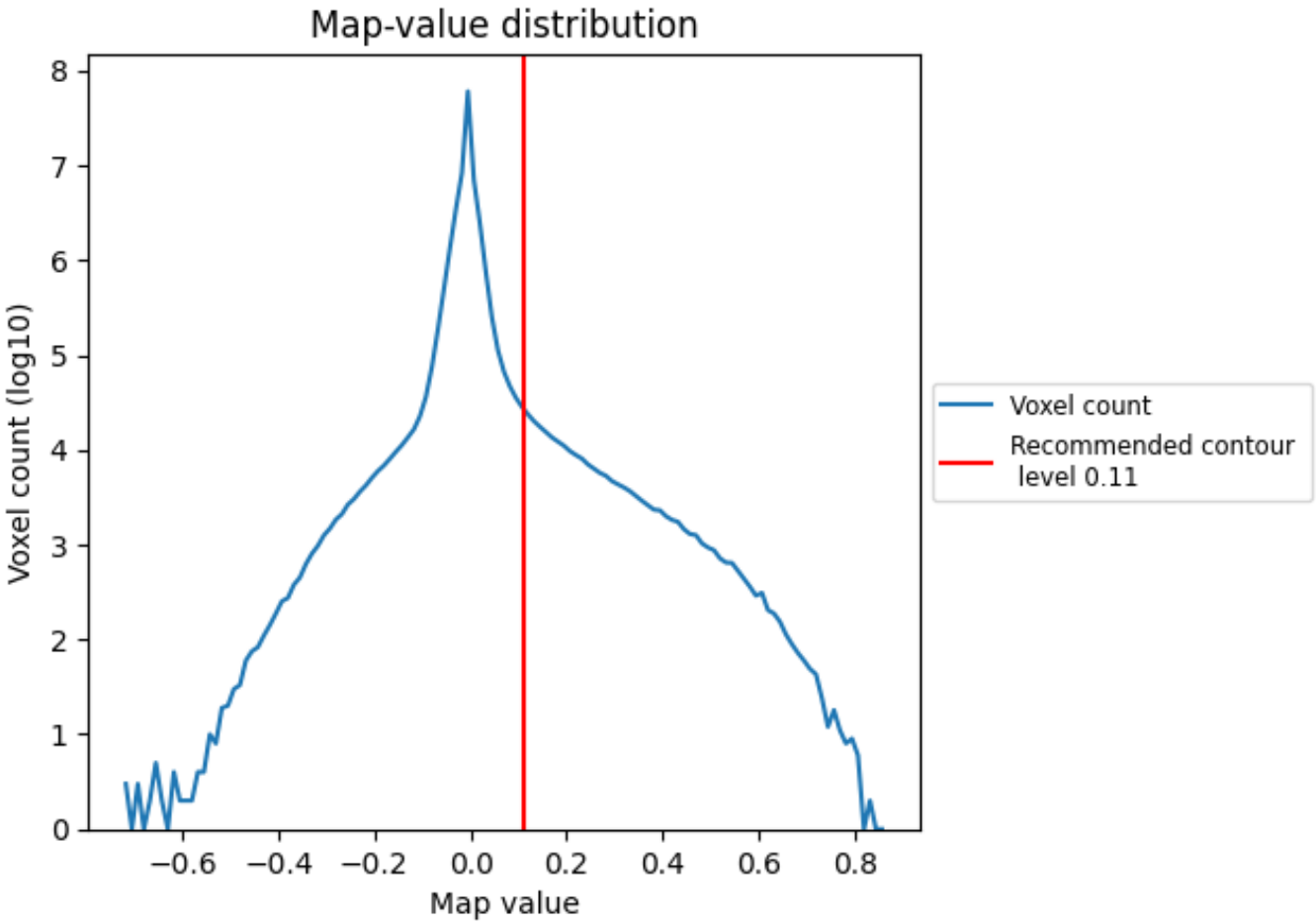
6.6 Mask visualisation (i)

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

7 Map analysis

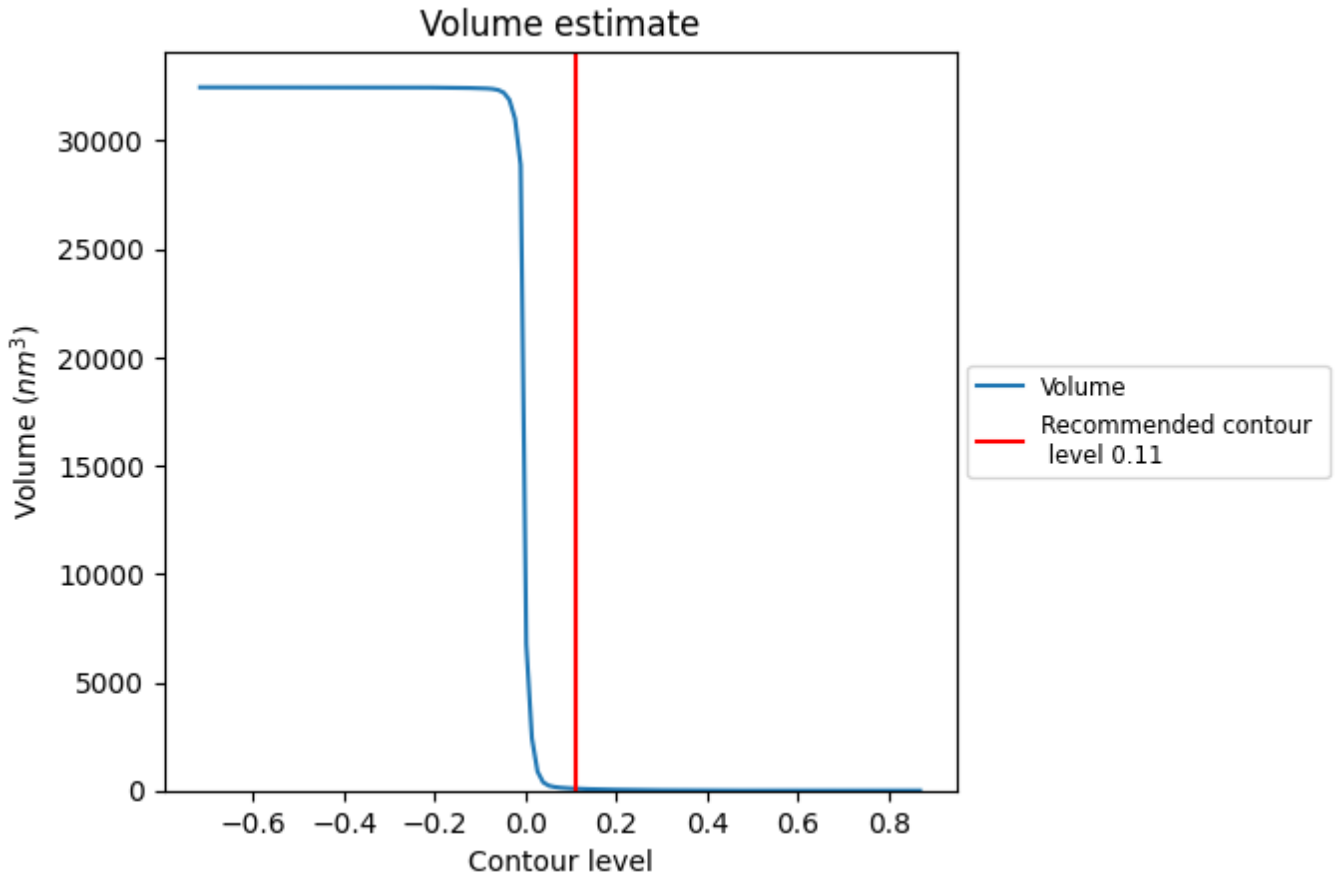
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

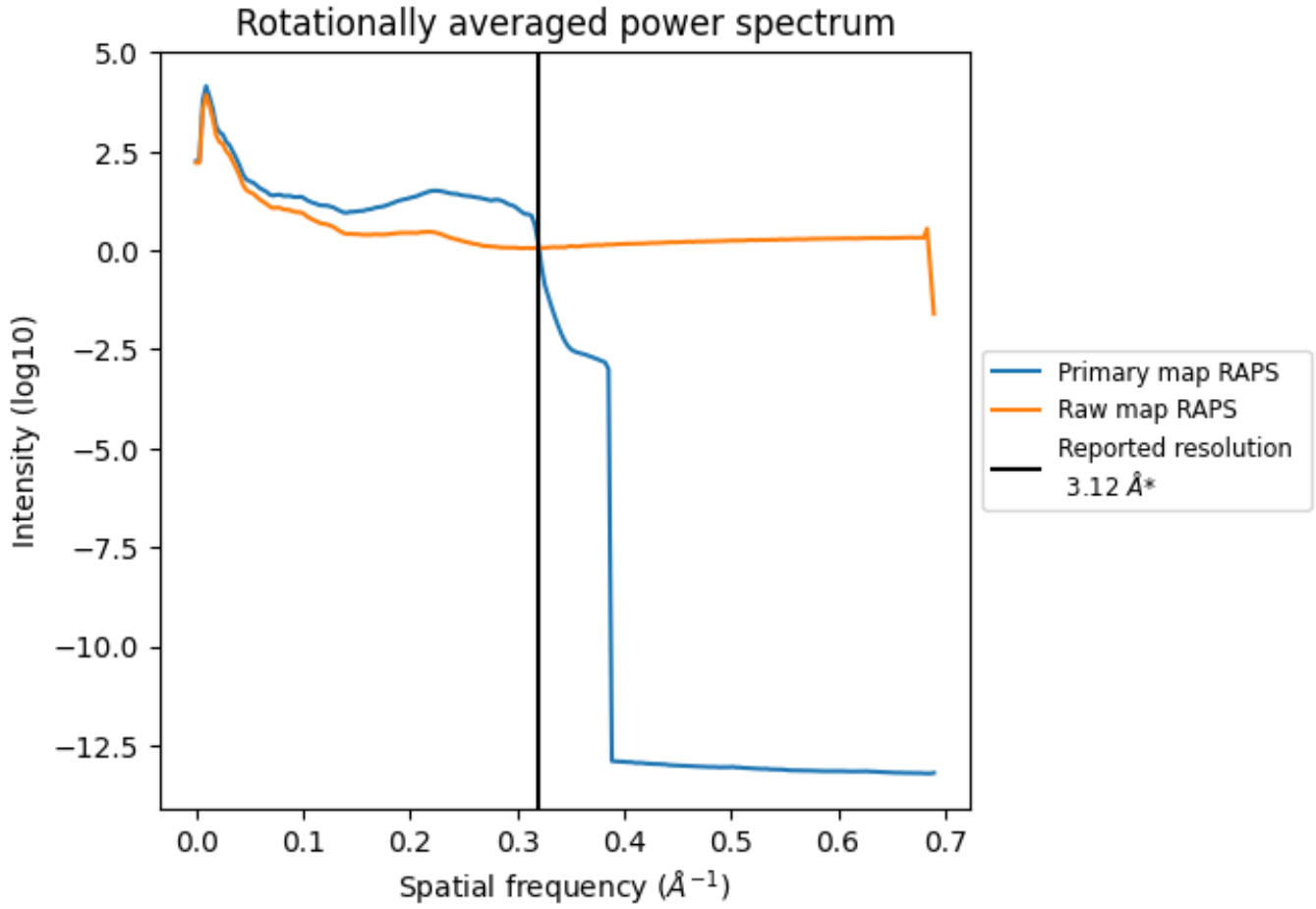
7.2 Volume estimate (i)



The volume at the recommended contour level is 89 nm^3; this corresponds to an approximate mass of 80 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)

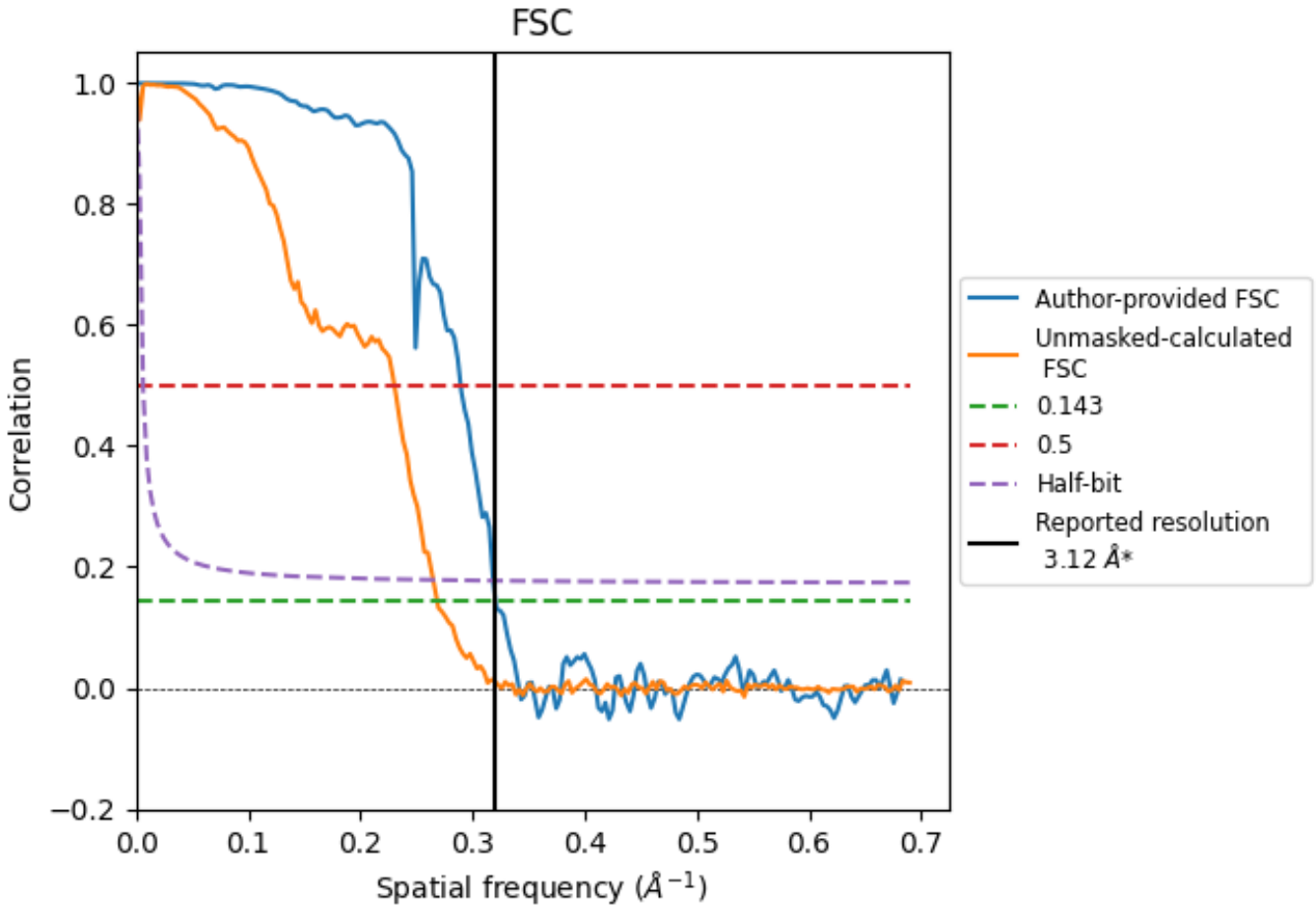


*Reported resolution corresponds to spatial frequency of 0.321 Å^{-1}

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 0.321 Å^{-1}

8.2 Resolution estimates (i)

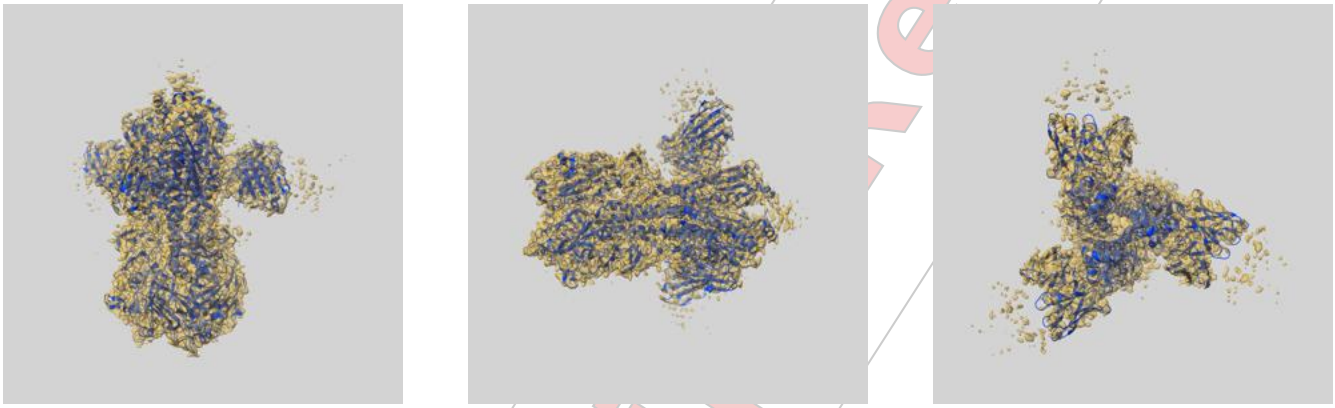
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	3.12	3.46	3.14
Unmasked-calculated*	3.72	4.34	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.72 differs from the reported value 3.12 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70236 and PDB model 9O8T. Per-residue inclusion information can be found in section 3 on page 11.

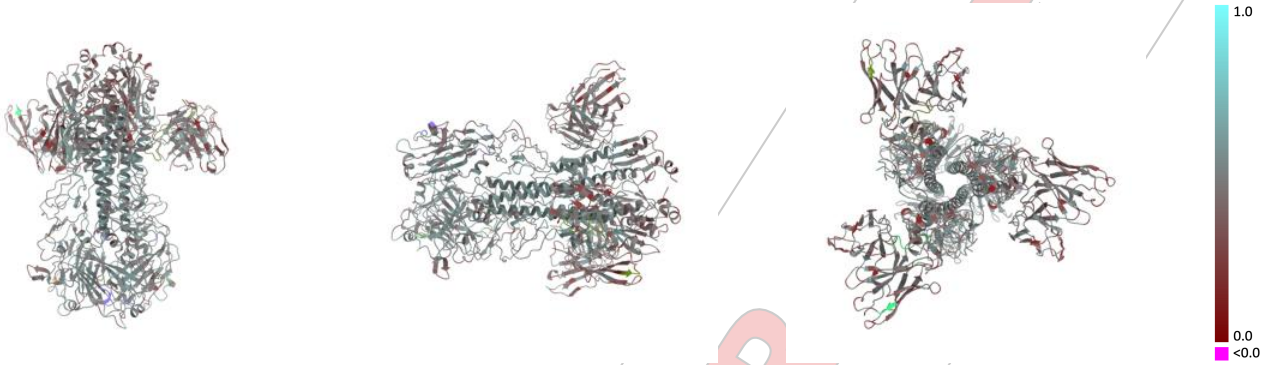
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

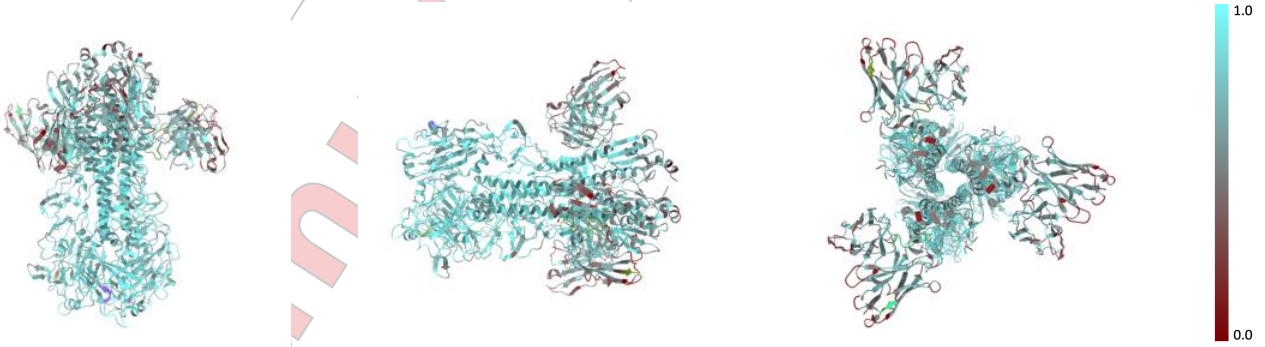
9.2 Q-score mapped to coordinate model



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.

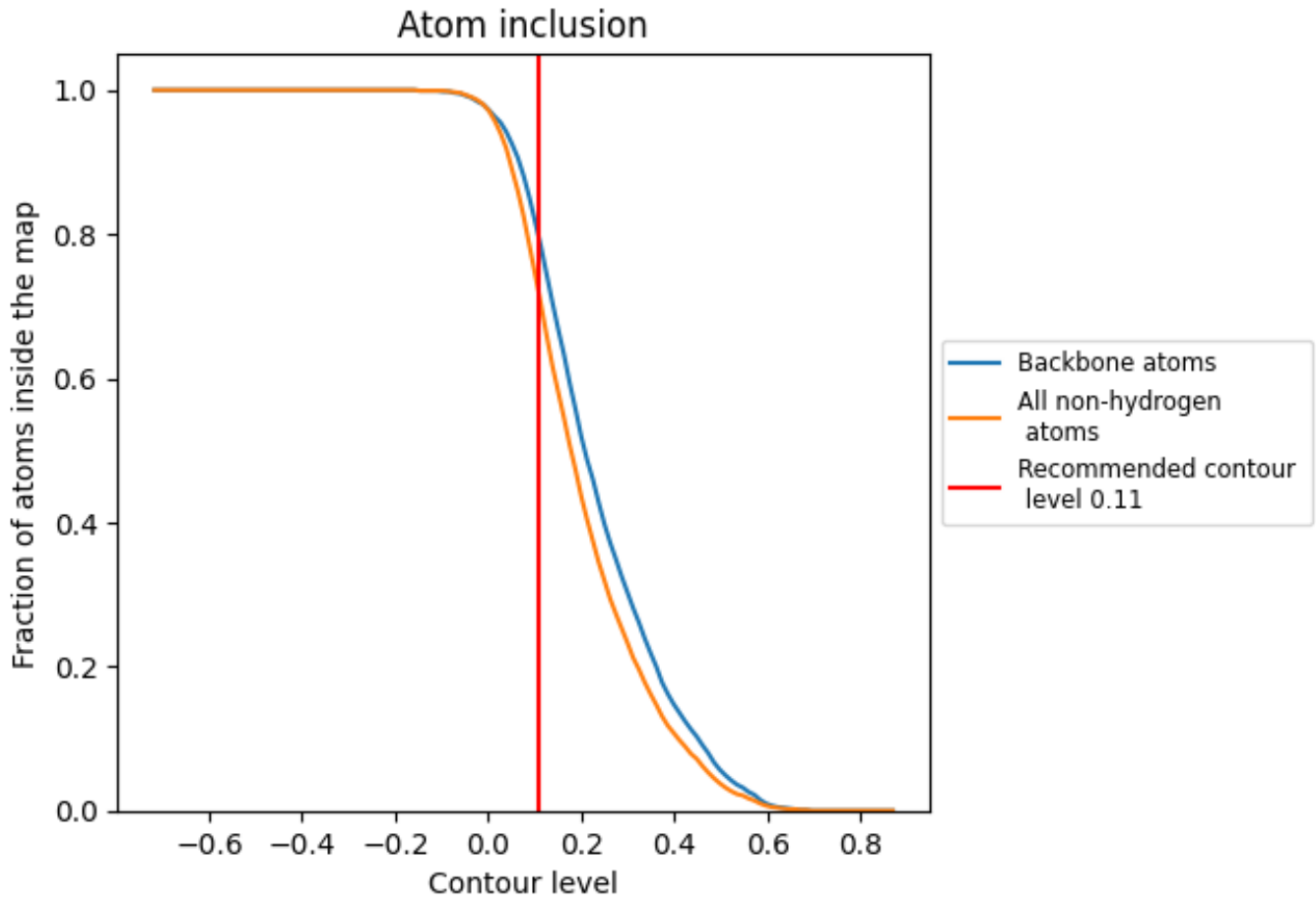
9.3 Atom inclusion mapped to coordinate model



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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.4720
A	0.7990	0.4990
B	0.7370	0.4900
C	0.7980	0.5000
D	0.7990	0.5000
E	0.7360	0.4910
F	0.7370	0.4890
G	0.5760	0.4220
H	0.5740	0.4190
I	0.5710	0.4240
J	0.5710	0.4130
K	0.5710	0.4150
L	0.5710	0.4140
M	0.5000	0.4230
N	0.5000	0.4250
O	0.5000	0.4180

Full wwPDB EM Validation Report (i)

May 6, 2025 – 10:29 AM EDT

PDB ID	:	9OI2 / pdb_00009oi2
EMDB ID	:	EMD-70502
Title	:	Structure of human Fab 245 in complex with influenza H1N1 A/Solomon Island/3/2006 hemagglutinin
Deposited on	:	2025-05-06
Resolution	:	2.80 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

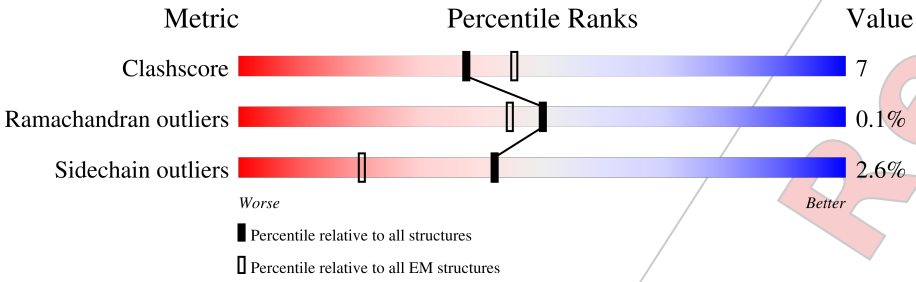
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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.



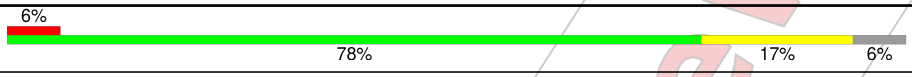
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 >=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	326	83% 15%
1	C	326	83% 14%
1	E	326	77% 20%
2	B	222	63% 12% 24%
2	D	222	64% 11% 24%
2	F	222	63% 13% 24%
3	H	138	75% 17% 7%
3	I	138	8% 71% 22% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	J	107	
4	L	107	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14649 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	322	Total	C	N	O	S	0	0
			2415	1531	428	445	11		
1	C	319	Total	C	N	O	S	0	0
			2382	1511	423	437	11		
1	E	320	Total	C	N	O	S	0	0
			2392	1517	424	441	10		

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	169	Total	C	N	O	S	0	0
			1334	838	232	257	7		
2	D	169	Total	C	N	O	S	0	0
			1326	833	230	256	7		
2	F	169	Total	C	N	O	S	0	0
			1330	835	231	257	7		

- Molecule 3 is a protein called Heavy chain of Fab from human antibody 245.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	129	Total	C	N	O	S	0	0
			969	612	165	187	5		
3	I	129	Total	C	N	O	S	0	0
			969	612	165	187	5		

- Molecule 4 is a protein called Light chain of Fab from human antibody 245.

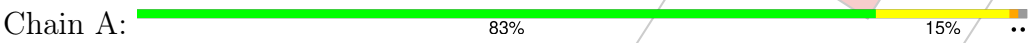
Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	101	Total	C	N	O	S	0	0
			766	479	134	151	2		
4	L	101	Total	C	N	O	S	0	0
			766	479	134	151	2		

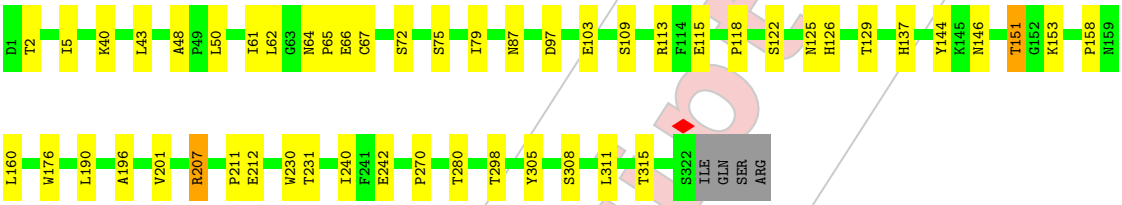
3 Residue-property plots (i)

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: Hemagglutinin HA1

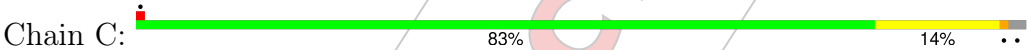
Chain A:

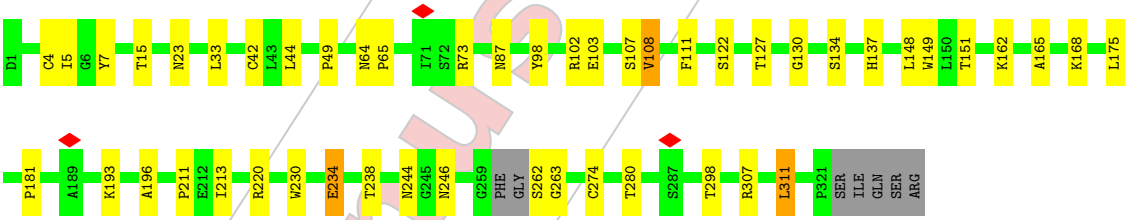




- Molecule 1: Hemagglutinin HA1

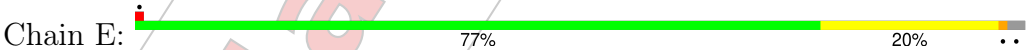
Chain C:

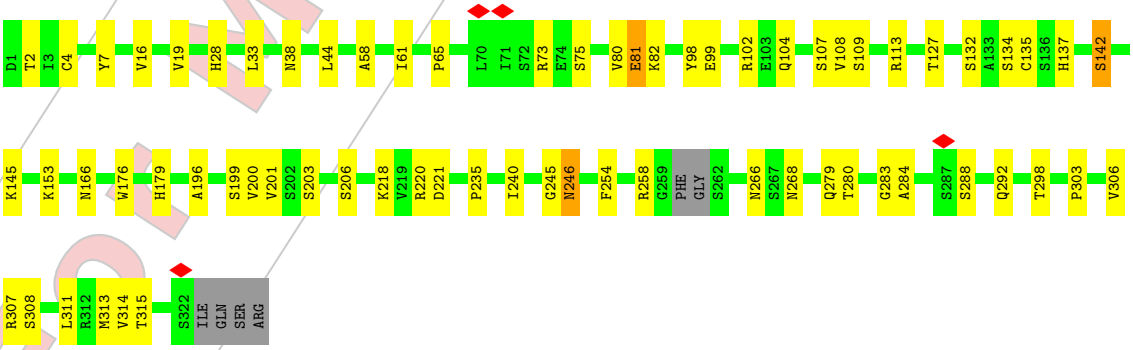




- Molecule 1: Hemagglutinin HA1

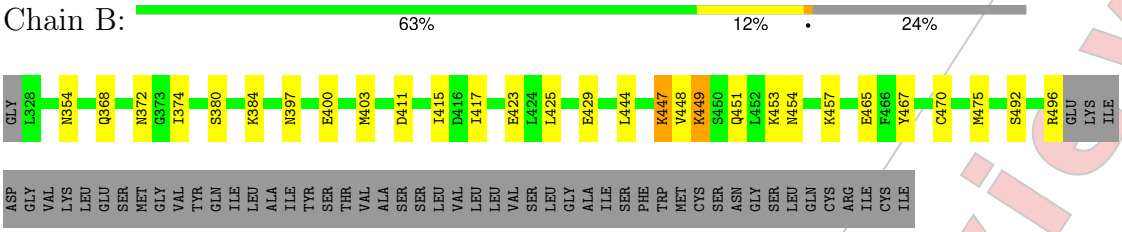
Chain E:





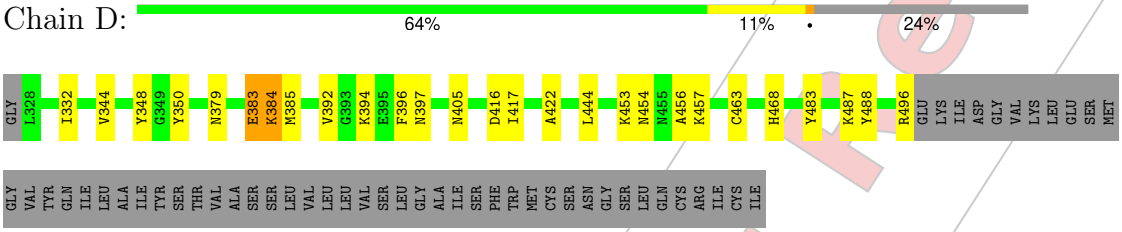
- Molecule 2: Hemagglutinin HA2

Chain B:



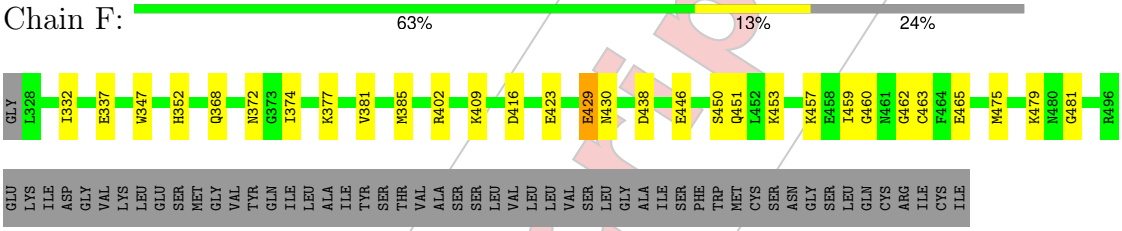
• Molecule 2: Hemagglutinin HA2

Chain D:



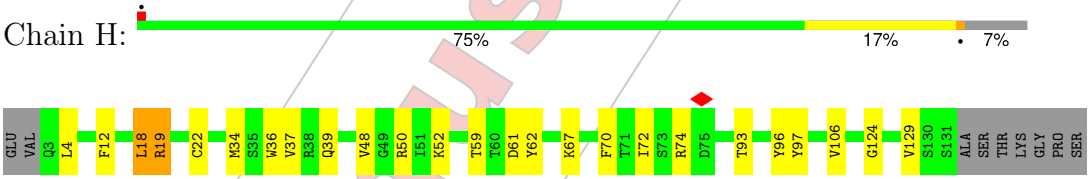
• Molecule 2: Hemagglutinin HA2

Chain F:



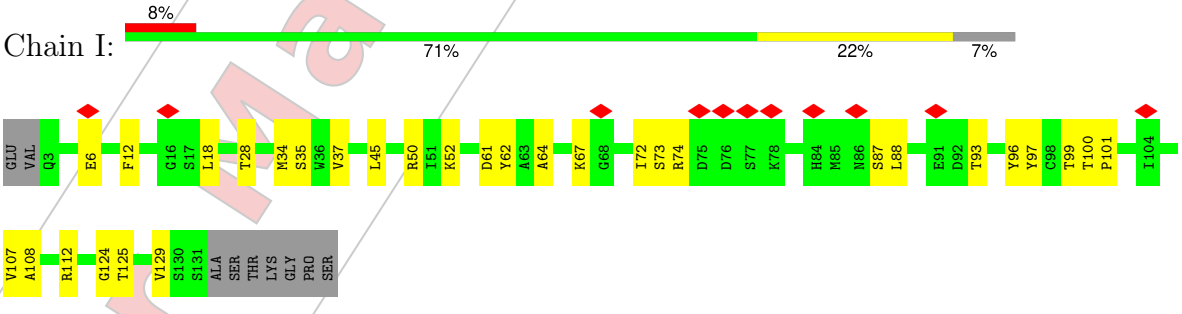
• Molecule 3: Heavy chain of Fab from human antibody 245

Chain H:



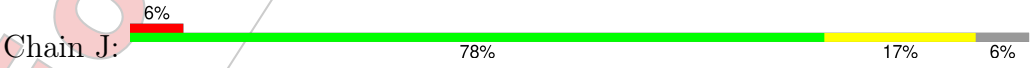
• Molecule 3: Heavy chain of Fab from human antibody 245

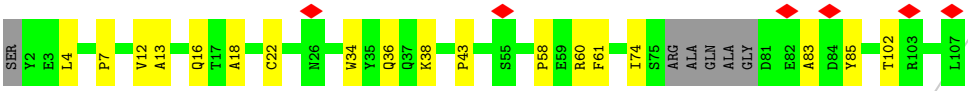
Chain I:



• Molecule 4: Light chain of Fab from human antibody 245

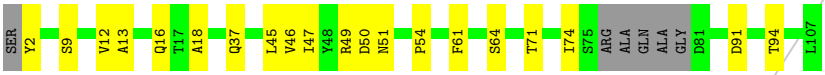
Chain J:





• Molecule 4: Light chain of Fab from human antibody 245

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256135	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.531	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	380.87997, 380.87997, 380.87997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.35	0/2480	0.56	0/3389
1	C	0.25	0/2446	0.39	0/3345
1	E	0.25	0/2456	0.38	0/3359
2	B	0.38	0/1361	0.60	0/1833
2	D	0.47	2/1353 (0.1%)	0.56	0/1824
2	F	0.23	0/1357	0.40	0/1829
3	H	0.22	0/993	0.41	0/1352
3	I	0.17	0/993	0.38	0/1352
4	J	0.14	0/782	0.32	0/1066
4	L	0.19	0/782	0.36	0/1066
All	All	0.29	2/15003 (0.0%)	0.46	0/20415

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
3	H	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	456	ALA	C-N	8.76	1.45	1.33
2	D	457	LYS	C-N	6.48	1.42	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ARG	Sidechain
3	H	19	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2278	30	0
1	C	2382	0	2228	30	0
1	E	2392	0	2241	45	0
2	B	1334	0	1250	21	0
2	D	1326	0	1233	22	0
2	F	1330	0	1239	30	0
3	H	969	0	921	19	0
3	I	969	0	921	19	0
4	J	766	0	734	12	0
4	L	766	0	734	13	0
All	All	14649	0	13779	207	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 7.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:CYS:HA	2:F:463:CYS:HB3	1.47	0.94
1:C:4:CYS:HA	2:D:463:CYS:HB3	1.62	0.82
4:L:13:ALA:HB3	4:L:16:GLN:HE22	1.45	0.79
4:L:16:GLN:N	4:L:16:GLN:OE1	2.18	0.77
1:E:104:GLN:OE1	1:E:258:ARG:NH2	2.19	0.74
1:E:134:SER:O	1:E:220:ARG:NH1	2.24	0.70
1:C:280:THR:HG22	1:C:298:THR:HG22	1.73	0.69
1:A:40:LYS:HG2	1:A:270:PRO:HG2	1.75	0.67
1:C:193:LYS:HE2	1:C:244:ASN:HB2	1.76	0.67
2:D:344:VAL:HG12	2:D:344:VAL:O	1.94	0.67
2:F:459:ILE:HD11	2:F:465:GLU:HB2	1.76	0.67
3:I:34:MET:HE3	3:I:34:MET:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:THR:HG1	1:C:151:THR:HG1	1.35	0.67
1:E:73:ARG:NH2	1:E:75:SER:O	2.27	0.67
1:E:218:LYS:HE2	1:E:221:ASP:HA	1.77	0.65
1:E:179:HIS:HB3	1:E:246:ASN:HB3	1.79	0.64
3:H:62:TYR:HE1	3:H:72:ILE:HG13	1.62	0.64
1:E:4:CYS:HA	2:F:463:CYS:CB	2.25	0.63
1:A:212:GLU:OE2	1:E:201:VAL:HG21	1.98	0.63
1:C:307:ARG:NH2	2:D:416:ASP:OD1	2.31	0.63
1:E:16:VAL:HG11	1:E:314:VAL:HG22	1.78	0.63
1:A:196:ALA:HB3	1:A:211:PRO:HG3	1.81	0.62
1:C:175:LEU:HD13	1:C:230:TRP:HB3	1.80	0.62
2:B:403:MET:HE3	2:B:403:MET:HA	1.81	0.62
2:D:394:LYS:NZ	2:F:409:LYS:HE2	2.14	0.62
1:A:65:PRO:HB2	1:A:137:HIS:HB2	1.82	0.61
2:F:451:GLN:HE22	2:F:481:GLY:HA2	1.65	0.61
1:A:151:THR:HG22	1:A:190:LEU:HB3	1.82	0.61
3:I:96:TYR:O	3:I:124:GLY:HA2	2.01	0.61
2:F:352:HIS:HB2	2:F:475:MET:HE3	1.82	0.60
1:C:4:CYS:HA	2:D:463:CYS:CB	2.31	0.59
3:H:93:THR:HG22	3:H:129:VAL:H	1.67	0.59
1:C:122:SER:O	1:C:162:LYS:NZ	2.23	0.59
1:E:7:TYR:OH	2:F:332:ILE:O	2.17	0.58
3:H:12:PHE:CZ	3:H:18:LEU:HG	2.38	0.58
1:A:315:THR:HG23	2:B:374:ILE:HG21	1.86	0.58
3:I:35:SER:OG	3:I:99:THR:OG1	2.22	0.57
1:A:125:ASN:HB3	1:A:158:PRO:HG2	1.85	0.57
1:E:196:ALA:HB1	1:E:245:GLY:HA3	1.87	0.56
1:A:308:SER:OG	2:B:423:GLU:OE2	2.13	0.56
1:E:33:LEU:HD13	1:E:311:LEU:HD12	1.88	0.56
1:E:268:ASN:OD1	1:E:268:ASN:N	2.40	0.55
1:E:292:GLN:HG2	1:E:303:PRO:HG2	1.87	0.55
3:I:100:THR:HG22	3:I:101:PRO:O	2.07	0.55
1:E:315:THR:HG23	2:F:374:ILE:HG21	1.87	0.55
1:E:218:LYS:CE	1:E:221:ASP:HA	2.36	0.55
4:L:12:VAL:HG21	4:L:18:ALA:HB2	1.88	0.55
1:C:103:GLU:HG2	2:F:402:ARG:HG3	1.88	0.55
1:E:201:VAL:HG22	1:E:206:SER:HB2	1.89	0.54
3:I:93:THR:HG22	3:I:129:VAL:H	1.71	0.54
1:A:97:ASP:HB2	1:A:230:TRP:HE1	1.73	0.54
1:C:262:SER:OG	1:C:263:GLY:N	2.39	0.53
1:E:246:ASN:OD1	1:E:246:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:HB3	1:A:67:CYS:HB2	1.89	0.53
4:L:46:VAL:HG12	4:L:47:ILE:HG13	1.90	0.53
1:C:98:TYR:O	1:C:102:ARG:HG3	2.08	0.53
2:F:451:GLN:NE2	2:F:481:GLY:HA2	2.23	0.53
3:I:50:ARG:NH2	3:I:61:ASP:OD2	2.41	0.53
2:B:400:GLU:O	2:B:403:MET:HB2	2.08	0.53
1:E:65:PRO:HA	1:E:145:LYS:HZ2	1.73	0.53
4:J:12:VAL:HG21	4:J:18:ALA:HB2	1.89	0.53
2:B:425:LEU:HG	2:B:429:GLU:OE2	2.09	0.53
1:E:279:GLN:NE2	1:E:283:GLY:O	2.42	0.53
1:E:113:ARG:HG3	1:E:254:PHE:CE1	2.44	0.52
1:E:38:ASN:HD21	1:E:284:ALA:HB3	1.74	0.52
1:E:313:MET:HE1	2:F:381:VAL:HG21	1.90	0.52
1:E:308:SER:OG	2:F:423:GLU:OE2	2.21	0.52
2:B:454:ASN:HD22	2:B:496:ARG:HH12	1.58	0.52
1:E:81:GLU:O	1:E:266:ASN:HA	2.09	0.52
3:H:96:TYR:O	3:H:124:GLY:HA2	2.09	0.52
1:C:107:SER:O	1:C:107:SER:OG	2.16	0.51
1:A:201:VAL:HG22	1:A:240:ILE:HB	1.92	0.51
1:C:311:LEU:HD21	2:D:422:ALA:HB1	1.93	0.51
1:A:115:GLU:OE2	1:A:118:PRO:HA	2.11	0.50
3:I:64:ALA:HA	3:I:67:LYS:HE2	1.93	0.50
1:E:28:HIS:CD2	3:I:108:ALA:HB2	2.47	0.50
1:E:306:VAL:HG21	1:E:311:LEU:HD11	1.93	0.50
1:A:280:THR:HG22	1:A:298:THR:HG22	1.91	0.50
2:B:368:GLN:HE22	4:L:49:ARG:HB3	1.77	0.49
2:B:444:LEU:HD12	2:B:447:LYS:HD2	1.93	0.49
1:C:181:PRO:HG2	1:C:213:ILE:HD12	1.94	0.49
3:H:36:TRP:HD1	3:H:72:ILE:HD13	1.77	0.49
3:I:37:VAL:HG13	3:I:97:TYR:HB2	1.94	0.49
1:A:160:LEU:O	1:A:242:GLU:HA	2.13	0.49
3:H:18:LEU:HD22	3:H:19:ARG:H	1.77	0.49
2:F:460:GLY:C	2:F:462:GLY:H	2.21	0.49
3:I:52:LYS:O	3:I:74:ARG:NH1	2.45	0.49
1:C:15:THR:HG23	1:C:23:ASN:HA	1.94	0.49
2:F:475:MET:O	2:F:479:LYS:HG3	2.12	0.49
3:H:62:TYR:O	3:H:67:LYS:NZ	2.46	0.49
1:A:5:ILE:HD11	2:B:448:VAL:HG21	1.96	0.48
2:B:417:ILE:HG21	2:D:417:ILE:HD13	1.94	0.48
1:E:135:CYS:HB2	1:E:142:SER:O	2.13	0.48
1:C:42:CYS:HB3	1:C:274:CYS:HB2	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:16:GLN:N	4:J:16:GLN:OE1	2.46	0.48
2:B:354:ASN:N	2:B:354:ASN:OD1	2.46	0.48
1:C:108:VAL:HG21	1:C:111:PHE:HB2	1.95	0.48
1:A:75:SER:OG	1:A:109:SER:O	2.24	0.48
1:A:103:GLU:OE2	2:D:405:ASN:ND2	2.44	0.48
2:B:380:SER:O	2:B:384:LYS:HG3	2.13	0.48
2:D:496:ARG:HE	2:D:496:ARG:HB3	1.50	0.48
1:E:65:PRO:HA	1:E:145:LYS:NZ	2.29	0.48
2:F:446:GLU:HA	2:F:446:GLU:OE1	2.13	0.48
3:I:62:TYR:HE1	3:I:72:ILE:HG13	1.79	0.48
4:L:45:LEU:HD23	4:L:54:PRO:HG3	1.94	0.47
1:A:64:ASN:ND2	1:A:66:GLU:HG2	2.29	0.47
1:C:7:TYR:OH	2:D:332:ILE:O	2.23	0.47
1:E:65:PRO:HB2	1:E:137:HIS:HB2	1.96	0.47
3:I:12:PHE:CD2	3:I:18:LEU:HD21	2.50	0.47
3:I:87:SER:O	3:I:87:SER:OG	2.29	0.47
2:D:396:PHE:HD1	2:F:402:ARG:HH21	1.62	0.47
4:L:64:SER:OG	4:L:71:THR:OG1	2.32	0.47
1:C:134:SER:O	1:C:220:ARG:NH1	2.48	0.46
3:H:62:TYR:CE1	3:H:72:ILE:HG13	2.47	0.46
1:A:305:TYR:CD2	2:B:415:ILE:HD13	2.51	0.46
1:E:166:ASN:HD22	1:E:235:PRO:HA	1.81	0.46
2:B:454:ASN:HB2	2:B:496:ARG:NH1	2.31	0.46
2:D:344:VAL:O	2:D:344:VAL:CG1	2.64	0.46
4:L:50:ASP:O	4:L:51:ASN:ND2	2.49	0.46
1:A:207:ARG:HE	1:A:207:ARG:HB3	1.56	0.45
1:E:280:THR:HG22	1:E:298:THR:HG22	1.97	0.45
2:F:457:LYS:HB3	2:F:457:LYS:HZ2	1.82	0.45
1:A:66:GLU:HG3	1:A:87:ASN:ND2	2.32	0.45
1:E:307:ARG:NH1	2:F:416:ASP:OD1	2.49	0.45
4:J:58:PRO:HB2	4:J:60:ARG:HG2	1.99	0.45
4:J:36:GLN:HB2	4:J:85:TYR:CE2	2.52	0.45
1:C:65:PRO:HB2	1:C:137:HIS:HB2	1.98	0.45
1:C:49:PRO:O	1:C:73:ARG:NH1	2.40	0.45
4:J:60:ARG:HG2	4:J:60:ARG:H	1.58	0.45
1:A:43:LEU:HD22	1:A:48:ALA:HA	1.99	0.45
2:F:385:MET:HB2	2:F:385:MET:HE2	1.78	0.45
3:H:37:VAL:HG13	3:H:97:TYR:HB2	1.99	0.45
2:F:332:ILE:N	2:F:438:ASP:OD2	2.49	0.45
2:B:368:GLN:HE21	2:B:372:ASN:HD21	1.64	0.44
4:J:13:ALA:HB3	4:J:16:GLN:NE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:HIS:CE1	2:F:347:TRP:HE1	2.35	0.44
3:I:6:GLU:HB2	3:I:125:THR:HG23	1.99	0.44
1:C:165:ALA:HA	1:C:238:THR:HG22	1.99	0.44
3:H:37:VAL:HA	3:H:48:VAL:HG23	2.00	0.44
1:A:118:PRO:O	1:A:122:SER:HB2	2.17	0.44
2:B:457:LYS:HG2	2:B:465:GLU:HB3	2.00	0.44
2:D:384:LYS:HD3	2:F:423:GLU:HB3	2.00	0.44
1:A:50:LEU:HD23	1:A:79:ILE:HG12	1.98	0.44
1:E:314:VAL:HG23	2:F:430:ASN:CG	2.43	0.44
2:B:470:CYS:SG	2:B:475:MET:HE2	2.57	0.44
4:L:12:VAL:HG11	4:L:18:ALA:HA	2.00	0.44
2:B:411:ASP:O	2:B:415:ILE:HG13	2.17	0.44
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.86	0.43
1:C:196:ALA:HB3	1:C:211:PRO:HG2	2.00	0.43
2:F:377:LYS:HE2	2:F:429:GLU:HG2	2.00	0.43
2:B:467:TYR:O	2:B:492:SER:HA	2.18	0.43
1:E:176:TRP:CE2	1:E:200:VAL:HG21	2.53	0.43
4:L:61:PHE:HE1	4:L:74:ILE:HG23	1.84	0.43
2:B:368:GLN:HE21	2:B:372:ASN:ND2	2.16	0.43
1:E:132:SER:C	1:E:134:SER:H	2.26	0.43
1:C:211:PRO:HG3	1:C:246:ASN:HB2	2.00	0.43
1:A:61:ILE:HD12	1:A:61:ILE:HA	1.91	0.43
2:F:450:SER:O	2:F:453:LYS:HD3	2.18	0.43
3:I:28:THR:O	3:I:28:THR:OG1	2.36	0.43
3:I:45:LEU:HD21	4:J:43:PRO:HG3	2.01	0.43
3:H:52:LYS:HE3	3:H:59:THR:HB	2.01	0.43
2:D:392:VAL:O	2:D:392:VAL:HG12	2.18	0.43
1:E:28:HIS:HD2	3:I:108:ALA:HB2	1.83	0.43
3:I:107:VAL:HG23	3:I:112:ARG:HG3	2.01	0.43
1:E:99:GLU:HA	1:E:102:ARG:HG3	2.01	0.42
4:J:22:CYS:HB2	4:J:34:TRP:CH2	2.53	0.42
3:H:4:LEU:HD22	3:H:22:CYS:SG	2.59	0.42
3:H:34:MET:HA	3:H:34:MET:HE2	2.01	0.42
2:D:350:TYR:OH	2:D:444:LEU:HD11	2.19	0.42
1:C:64:ASN:ND2	1:C:87:ASN:HB3	2.34	0.42
1:C:130:GLY:HA3	1:C:149:TRP:HB3	2.02	0.42
3:H:39:GLN:OE1	4:L:37:GLN:NE2	2.29	0.42
4:J:38:LYS:HG2	4:J:83:ALA:HB2	1.99	0.42
1:C:64:ASN:HD22	1:C:87:ASN:HB3	1.84	0.42
1:E:127:THR:HG23	1:E:153:LYS:HA	2.01	0.42
4:J:61:PHE:HE1	4:J:74:ILE:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:394:LYS:HZ3	2:F:409:LYS:HE2	1.84	0.42
3:H:18:LEU:HD22	3:H:19:ARG:N	2.35	0.42
1:A:113:ARG:NH1	1:A:146:ASN:OD1	2.53	0.41
1:C:234:GLU:H	1:C:234:GLU:HG3	1.67	0.41
4:J:7:PRO:O	4:J:102:THR:OG1	2.29	0.41
1:A:315:THR:HG21	3:H:106:VAL:HA	2.02	0.41
2:D:379:ASN:O	2:D:383:GLU:HB2	2.20	0.41
2:D:487:LYS:HD3	2:D:488:TYR:CE1	2.56	0.41
2:B:449:LYS:HB3	2:B:449:LYS:HE3	1.62	0.41
3:H:50:ARG:NH2	3:H:61:ASP:OD2	2.54	0.41
3:H:52:LYS:O	3:H:74:ARG:NH1	2.52	0.41
4:L:50:ASP:C	4:L:51:ASN:ND2	2.79	0.41
1:A:62:LEU:O	1:A:144:TYR:HB3	2.21	0.41
3:I:88:LEU:HD23	3:I:129:VAL:HG22	2.03	0.41
1:C:73:ARG:HA	1:C:73:ARG:HD2	1.80	0.41
3:H:70:PHE:CD1	3:H:70:PHE:N	2.88	0.41
1:A:176:TRP:HZ3	1:A:231:THR:HG22	1.85	0.41
2:D:453:LYS:HB3	2:D:454:ASN:H	1.80	0.41
2:F:337:GLU:H	2:F:337:GLU:HG2	1.56	0.41
4:J:4:LEU:HD13	4:J:22:CYS:SG	2.60	0.41
4:L:2:TYR:HB2	4:L:91:ASP:OD2	2.21	0.41
1:E:28:HIS:HE1	2:F:347:TRP:HE1	1.67	0.41
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.91	0.40
1:E:58:ALA:HB2	1:E:98:TYR:CE1	2.56	0.40
1:E:61:ILE:HD12	1:E:61:ILE:HA	1.96	0.40
2:F:368:GLN:HE21	2:F:372:ASN:ND2	2.19	0.40
1:A:126:HIS:HE1	1:A:158:PRO:O	2.04	0.40
2:D:394:LYS:NZ	2:F:409:LYS:CE	2.82	0.40
2:D:468:HIS:NE2	2:D:483:TYR:OH	2.53	0.40
2:D:385:MET:HE2	2:D:385:MET:HB2	1.97	0.40
1:E:109:SER:OG	1:E:258:ARG:O	2.38	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	320/326 (98%)	302 (94%)	18 (6%)	0	100	100
1	C	315/326 (97%)	295 (94%)	20 (6%)	0	100	100
1	E	316/326 (97%)	301 (95%)	15 (5%)	0	100	100
2	B	167/222 (75%)	161 (96%)	5 (3%)	1 (1%)	22	51
2	D	167/222 (75%)	163 (98%)	4 (2%)	0	100	100
2	F	167/222 (75%)	164 (98%)	3 (2%)	0	100	100
3	H	127/138 (92%)	123 (97%)	4 (3%)	0	100	100
3	I	127/138 (92%)	125 (98%)	2 (2%)	0	100	100
4	J	97/107 (91%)	92 (95%)	5 (5%)	0	100	100
4	L	97/107 (91%)	93 (96%)	4 (4%)	0	100	100
All	All	1900/2134 (89%)	1819 (96%)	80 (4%)	1 (0%)	50	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	453	LYS

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	251/286 (88%)	245 (98%)	6 (2%)	44	77
1	C	245/286 (86%)	238 (97%)	7 (3%)	37	71
1	E	247/286 (86%)	234 (95%)	13 (5%)	19	49
2	B	138/191 (72%)	134 (97%)	4 (3%)	37	71
2	D	136/191 (71%)	132 (97%)	4 (3%)	37	71
2	F	137/191 (72%)	136 (99%)	1 (1%)	81	94
3	H	99/109 (91%)	98 (99%)	1 (1%)	73	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	99/109 (91%)	98 (99%)	1 (1%)	73 91
4	J	84/88 (96%)	84 (100%)	0	100 100
4	L	84/88 (96%)	82 (98%)	2 (2%)	44 77
All	All	1520/1825 (83%)	1481 (97%)	39 (3%)	42 75

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	72	SER
1	A	129	THR
1	A	151	THR
1	A	153	LYS
1	A	311	LEU
2	B	397	ASN
2	B	447	LYS
2	B	449	LYS
2	B	451	GLN
1	C	5	ILE
1	C	33	LEU
1	C	44	LEU
1	C	108	VAL
1	C	168	LYS
1	C	234	GLU
1	C	311	LEU
2	D	348	TYR
2	D	383	GLU
2	D	384	LYS
2	D	397	ASN
1	E	2	THR
1	E	19	VAL
1	E	80	VAL
1	E	81	GLU
1	E	82	LYS
1	E	107	SER
1	E	108	VAL
1	E	142	SER
1	E	199	SER
1	E	203	SER
1	E	240	ILE
1	E	246	ASN

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Mol	Chain	Res	Type
1	E	288	SER
2	F	429	GLU
3	H	18	LEU
3	I	73	SER
4	L	9	SER
4	L	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	279	GLN
2	B	368	GLN
2	B	386	ASN
2	B	397	ASN
2	B	454	ASN
1	C	84	ASN
1	C	126	HIS
1	C	266	ASN
2	D	451	GLN
1	E	28	HIS
2	F	353	GLN
2	F	368	GLN
2	F	372	ASN
2	F	376	ASN
2	F	451	GLN
3	H	39	GLN
3	H	84	HIS
3	I	84	HIS
4	J	52	ASN
4	L	37	GLN
4	L	52	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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

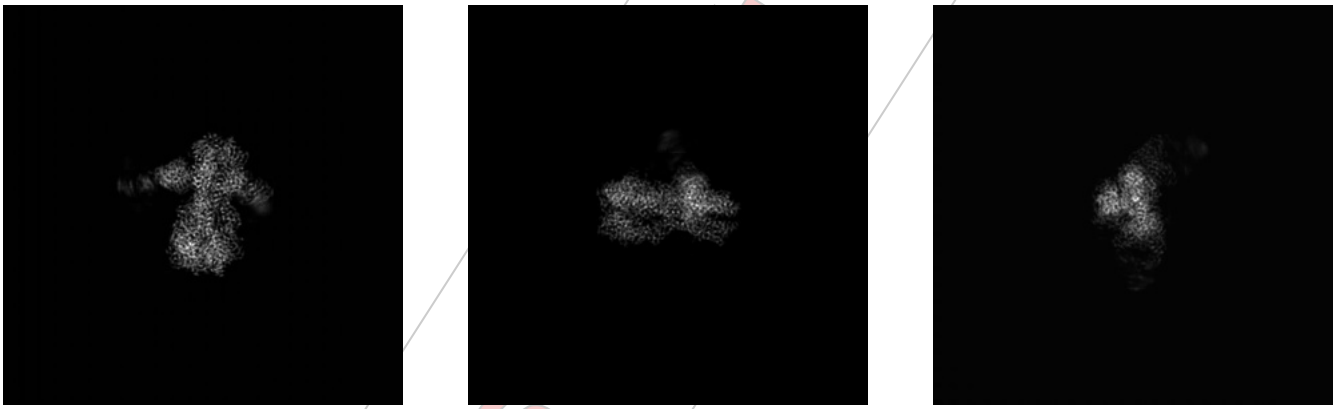
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70502. 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.

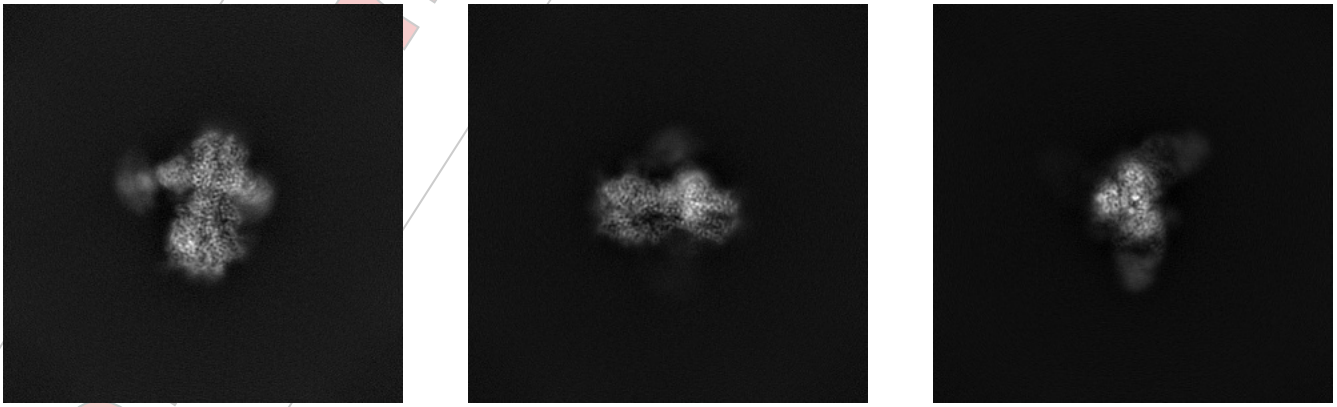
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

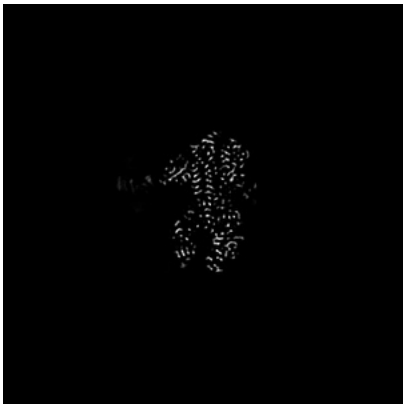


X Y Z

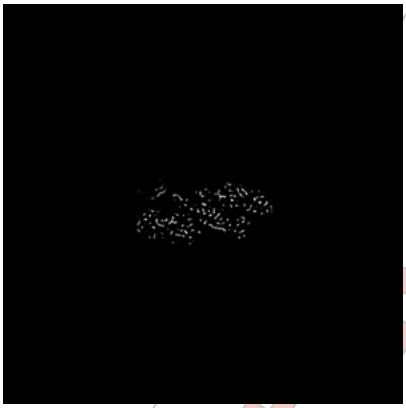
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



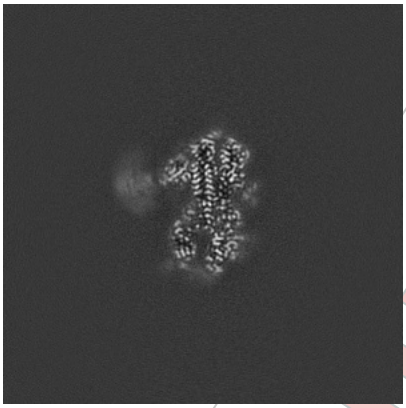
X Index: 180



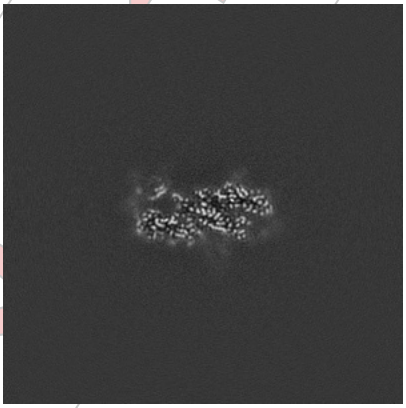
Y Index: 180

Z Index: 180

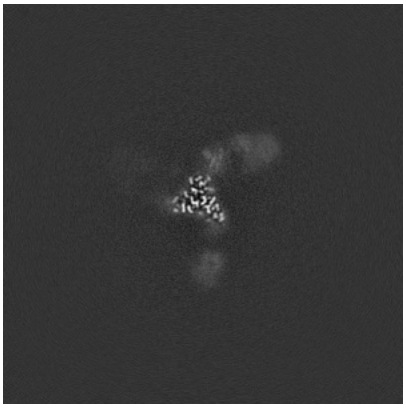
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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

6.3 Largest variance slices (i)

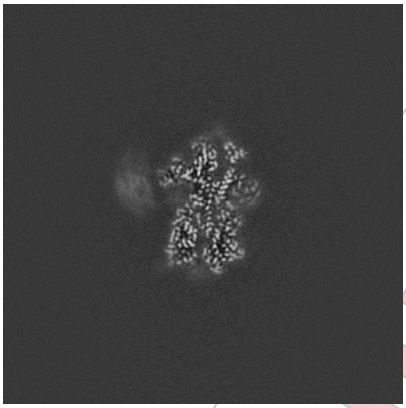
6.3.1 Primary map

X Index: 185

Y Index: 184

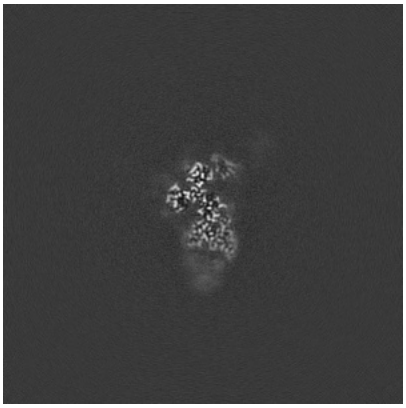
Z Index: 201

6.3.2 Raw map



X Index: 185

Y Index: 184

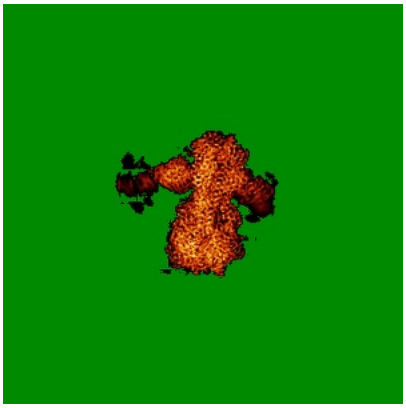


Z Index: 208

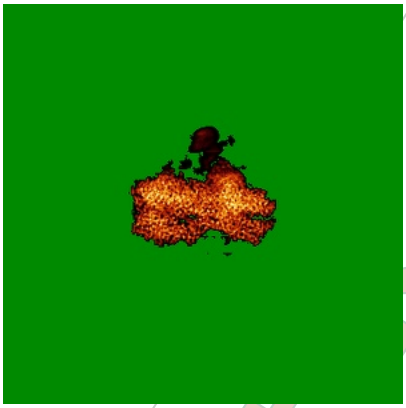
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

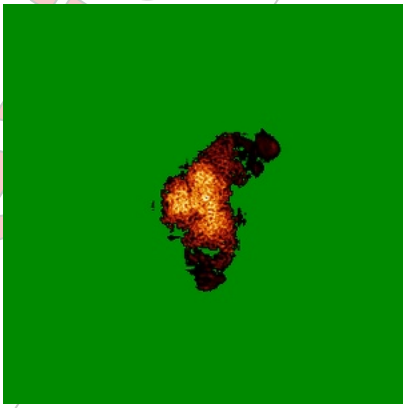
6.4.1 Primary map



X

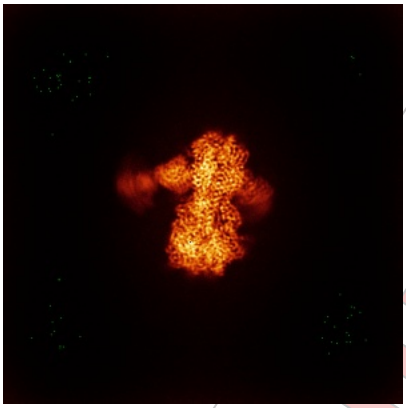


Y

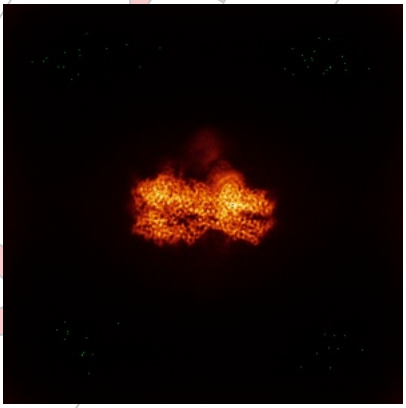


Z

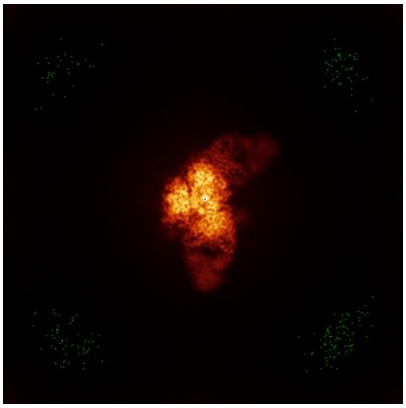
6.4.2 Raw map



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.

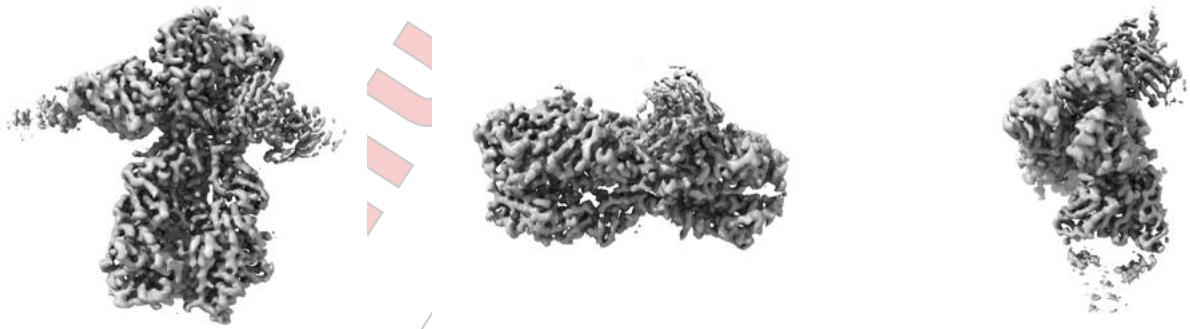
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

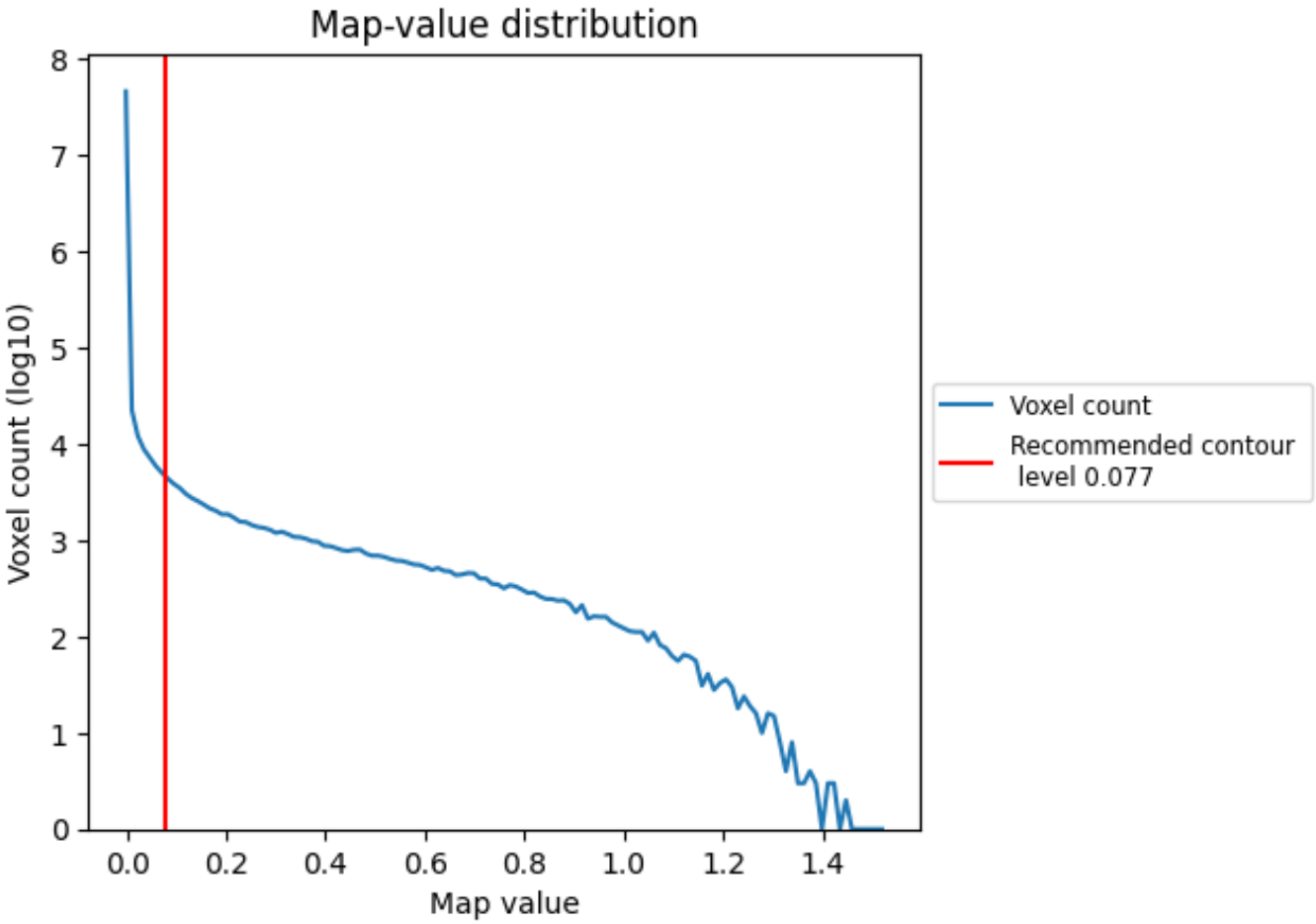
6.6 Mask visualisation (i)

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

7 Map analysis

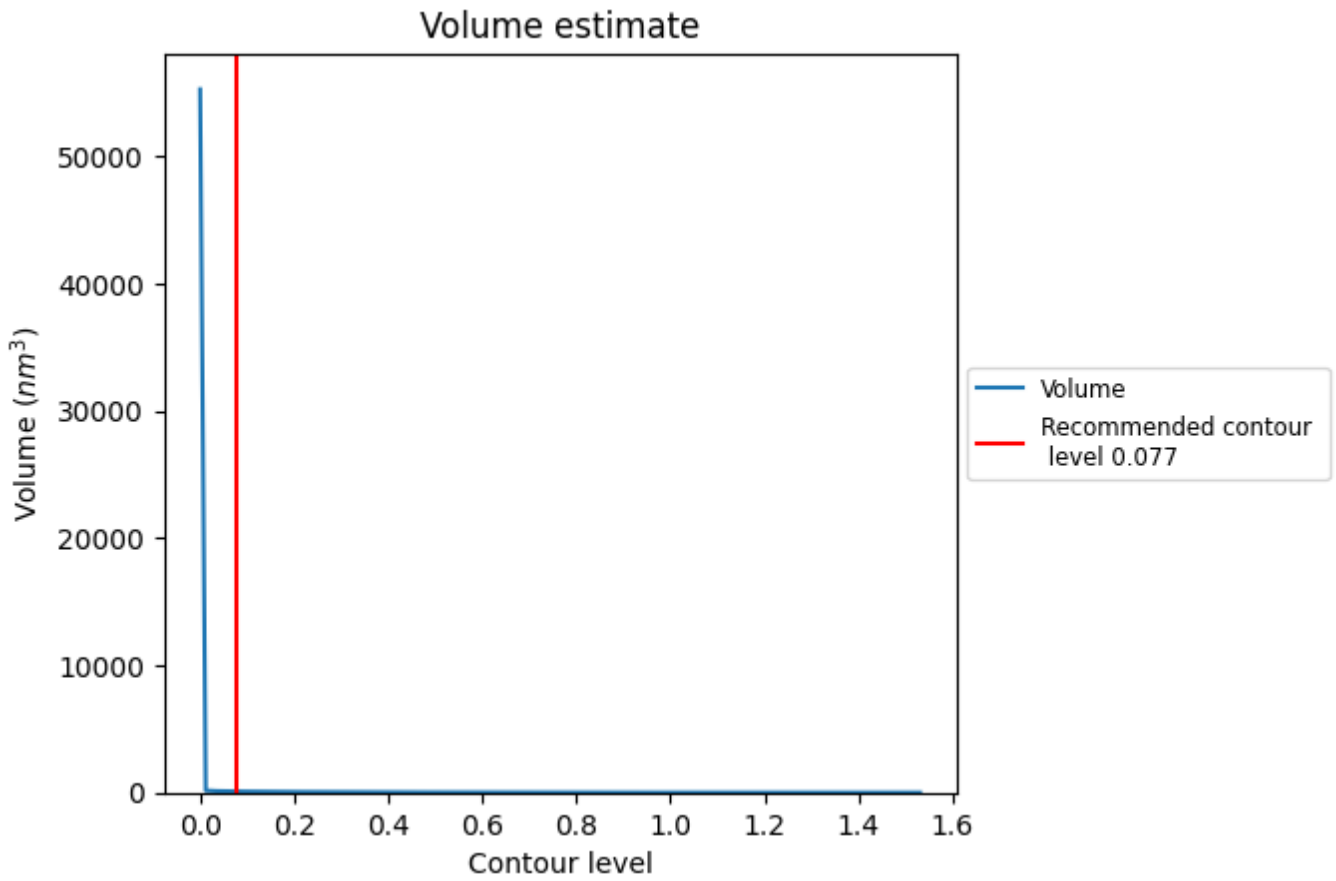
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

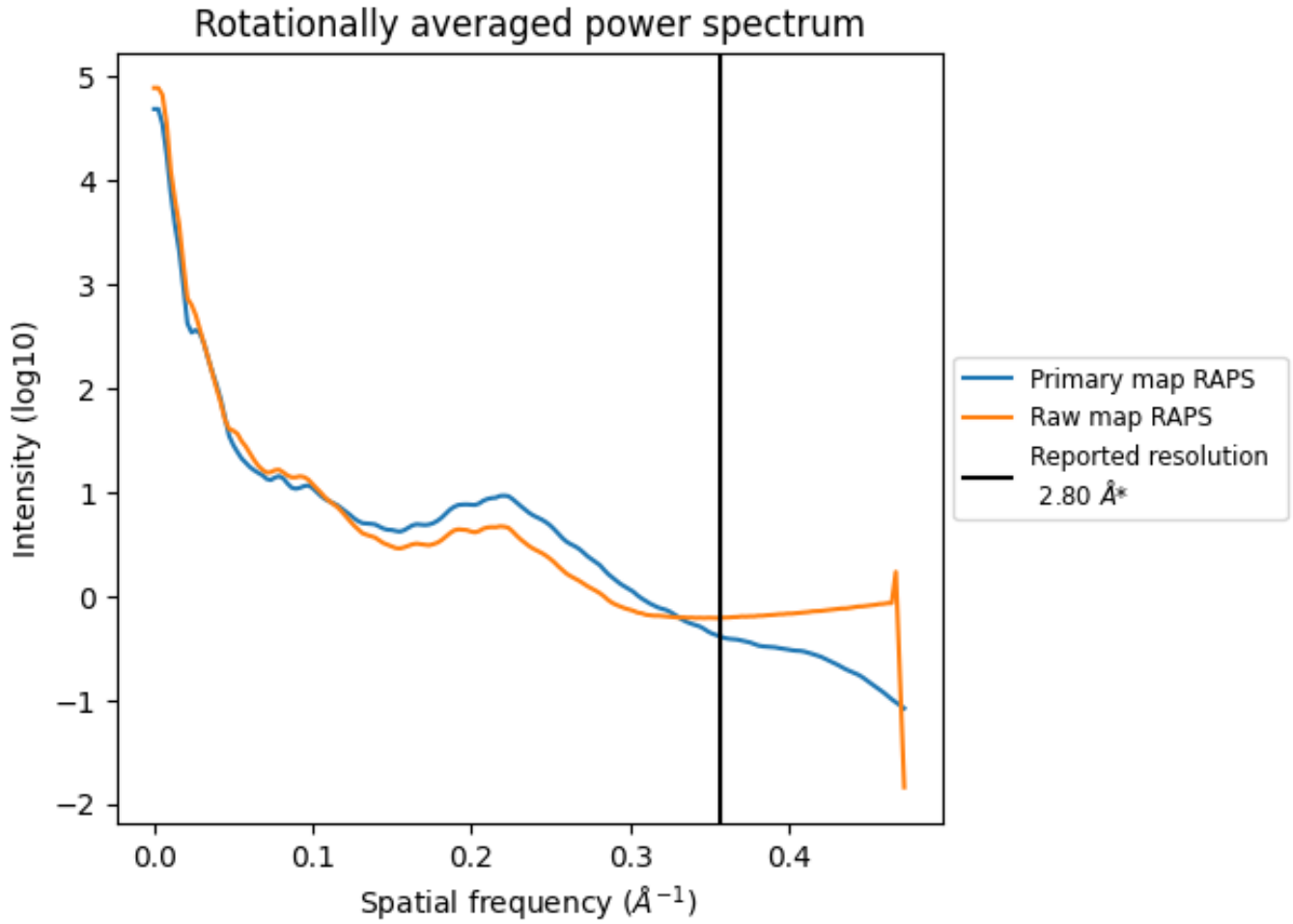
7.2 Volume estimate (i)



The volume at the recommended contour level is 90 nm^3; this corresponds to an approximate mass of 81 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)

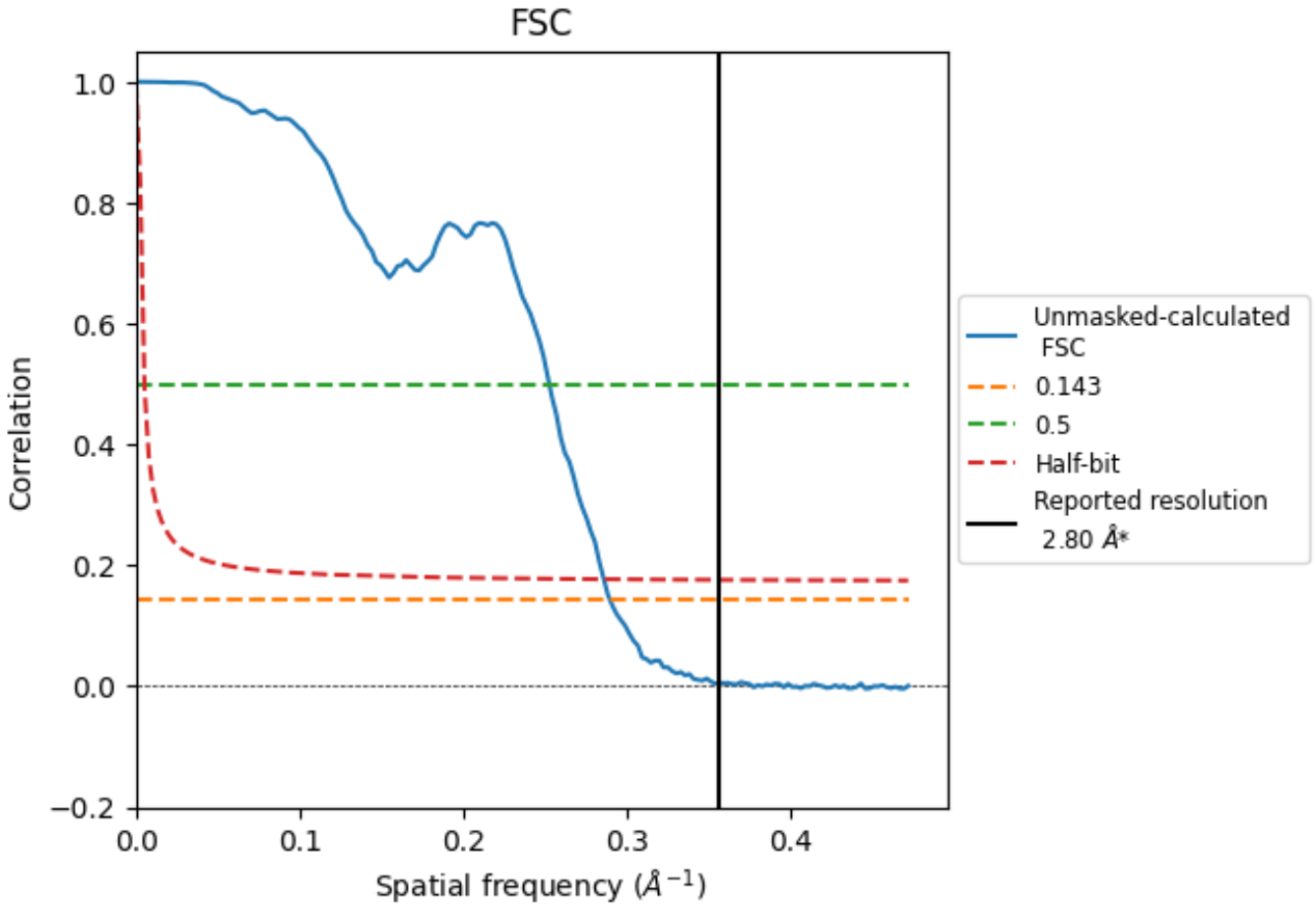


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

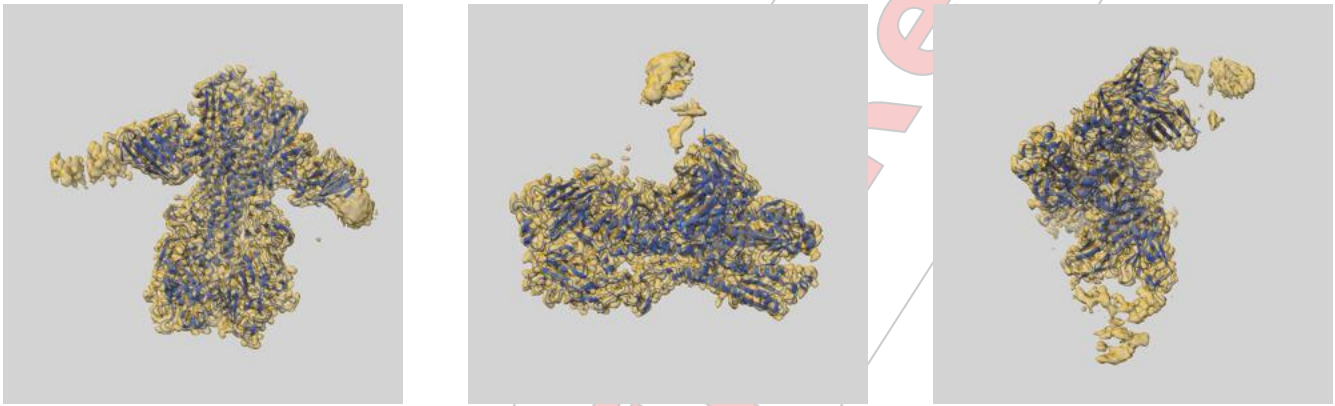
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	3.95	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 2.8 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70502 and PDB model 9OI2. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay



X Y Z

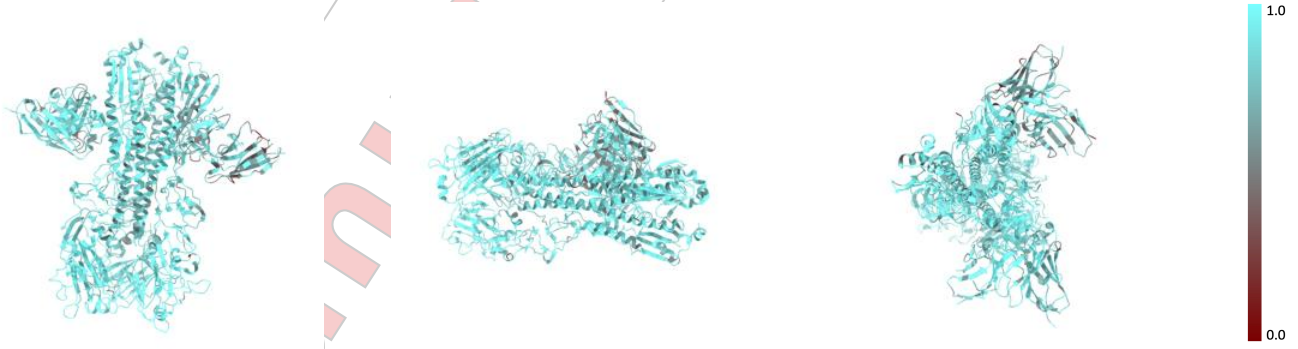
The images above show the 3D surface view of the map at the recommended contour level 0.077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

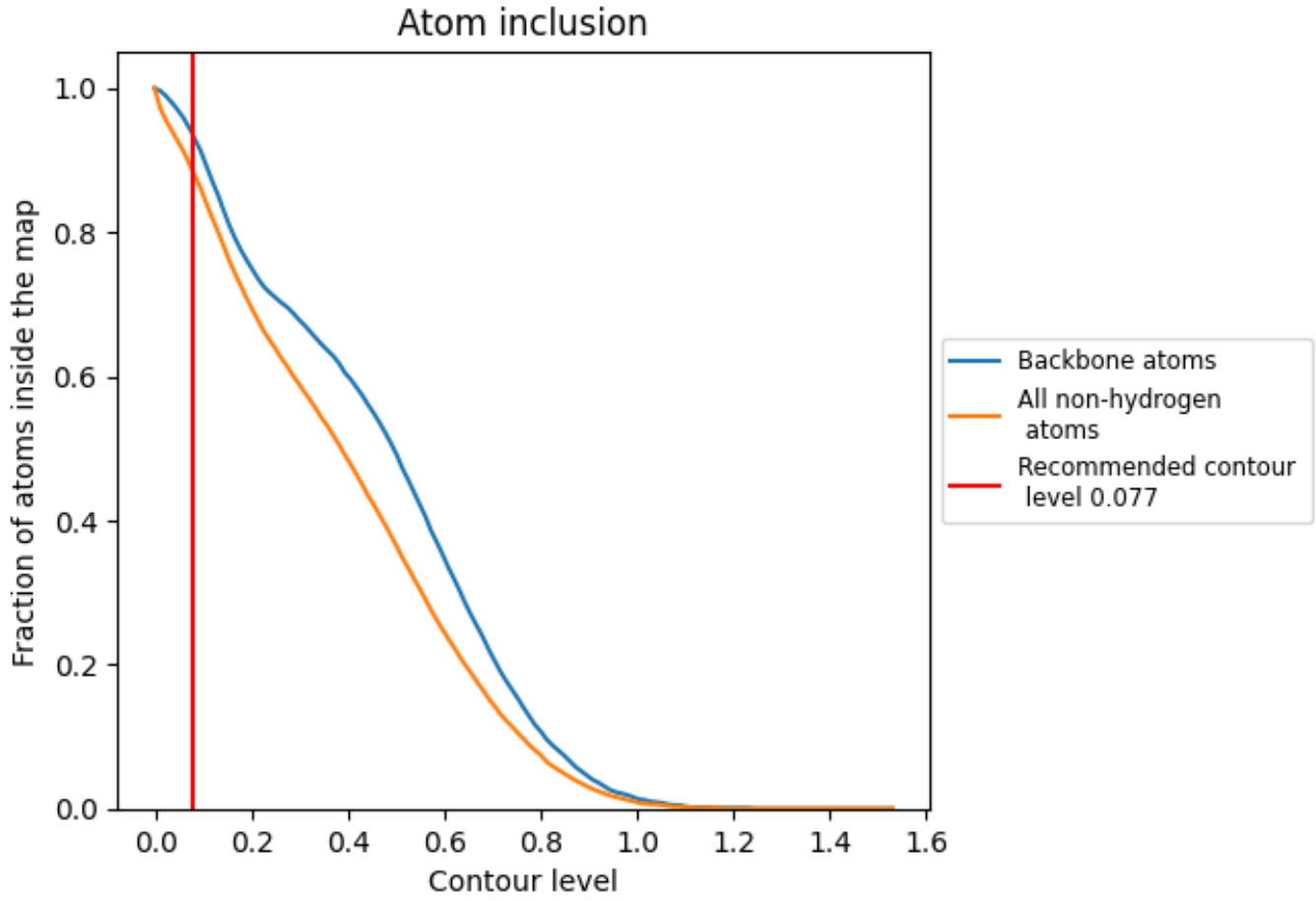
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.077).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8860	0.5530
A	0.9310	0.5820
B	0.9000	0.5690
C	0.9300	0.5770
D	0.8890	0.5550
E	0.9210	0.5720
F	0.9070	0.5720
H	0.8450	0.5190
I	0.7150	0.4480
J	0.7150	0.4570
L	0.8660	0.5340

Full wwPDB EM Validation Report (i)

May 6, 2025 – 10:29 AM EDT

PDB ID	:	9OI3 / pdb_00009oi3
EMDB ID	:	EMD-70503
Title	:	Structure of human Fab 604 in complex with influenza H1N1 A/Solomon Island/3/2006 hemagglutinin
Deposited on	:	2025-05-06
Resolution	:	2.71 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

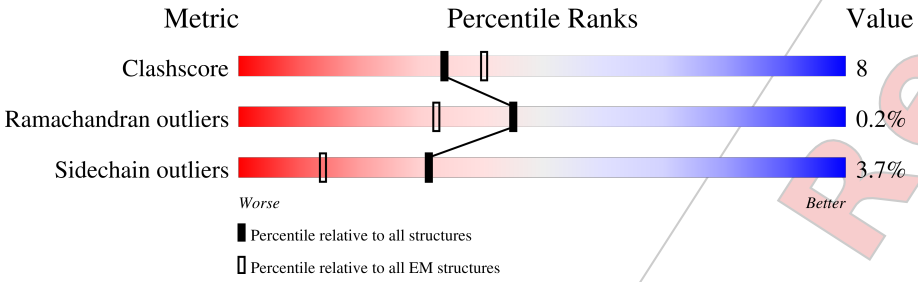
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.71 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	326	82% 15% • •
1	C	326	76% 19% • •
1	E	326	78% 19% • •
2	B	222	64% 11% • 24%
2	D	222	59% 16% • 24%
2	F	222	61% 14% • 24%
3	H	134	73% 21% • 5%
3	I	134	69% 21% • 8%

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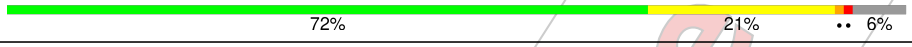
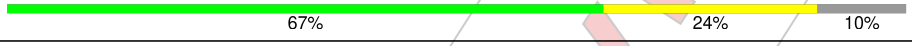
Mol	Chain	Length	Quality of chain
3	M	134	
4	J	114	
4	L	114	
4	N	114	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16485 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2428	1538	430	449	11		
1	C	319	Total	C	N	O	S	0	0
			2386	1514	424	437	11		
1	E	320	Total	C	N	O	S	0	0
			2401	1522	425	444	10		

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	169	Total	C	N	O	S	0	0
			1334	838	232	257	7		
2	D	169	Total	C	N	O	S	0	0
			1330	835	230	258	7		
2	F	169	Total	C	N	O	S	0	0
			1338	840	232	259	7		

- Molecule 3 is a protein called Heavy chain of Fab from human antibody 604.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	127	Total	C	N	O	S	0	0
			977	615	167	189	6		
3	I	123	Total	C	N	O	S	0	0
			953	601	163	183	6		
3	M	126	Total	C	N	O	S	0	0
			964	607	164	187	6		

- Molecule 4 is a protein called Light chain of Fab from human antibody 604.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	104	Total	C	N	O	S	0	0
			796	498	131	164	3		

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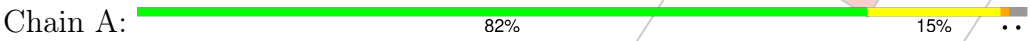
Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	103	Total	C	N	O	S	0	0
			788	494	130	161	3		
4	N	104	Total	C	N	O	S	0	0
			790	492	131	164	3		

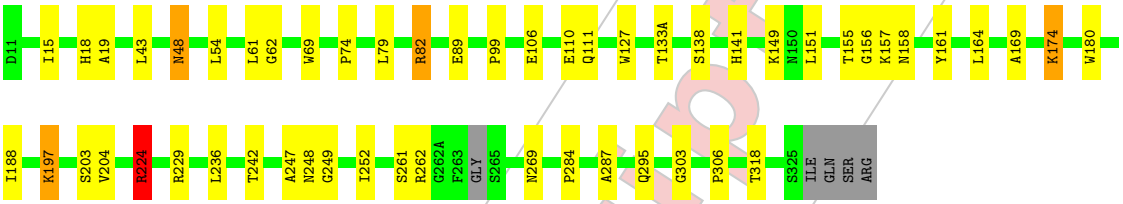
3 Residue-property plots (i)

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: Hemagglutinin HA1

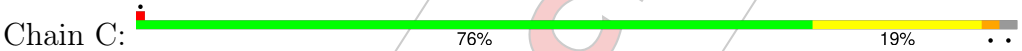
Chain A:





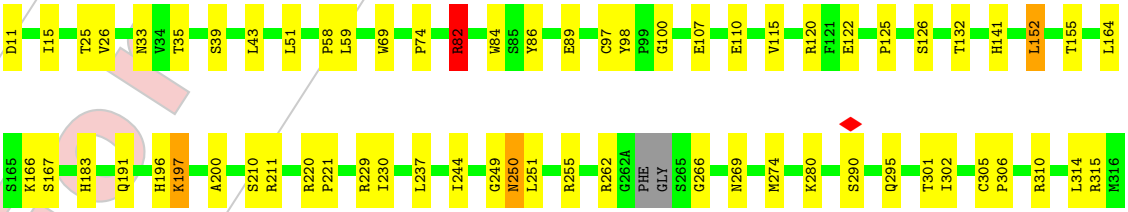
- Molecule 1: Hemagglutinin HA1

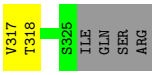
Chain C:



- Molecule 1: Hemagglutinin HA1

Chain E:



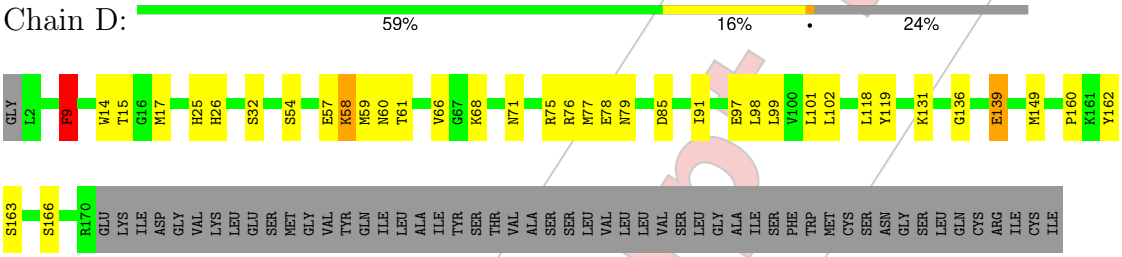


• Molecule 2: Hemagglutinin HA2

Chain B:

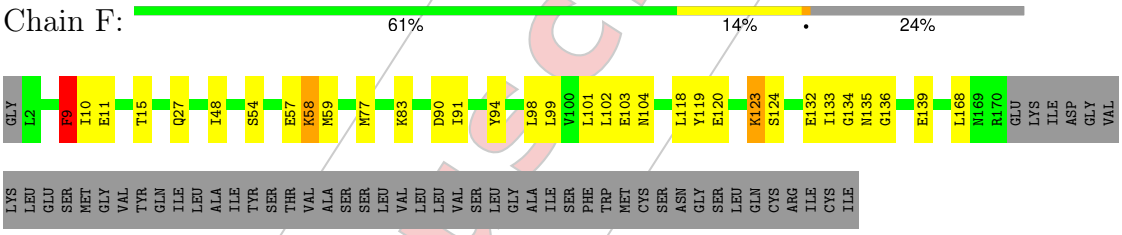
• Molecule 2: Hemagglutinin HA2

Chain D:



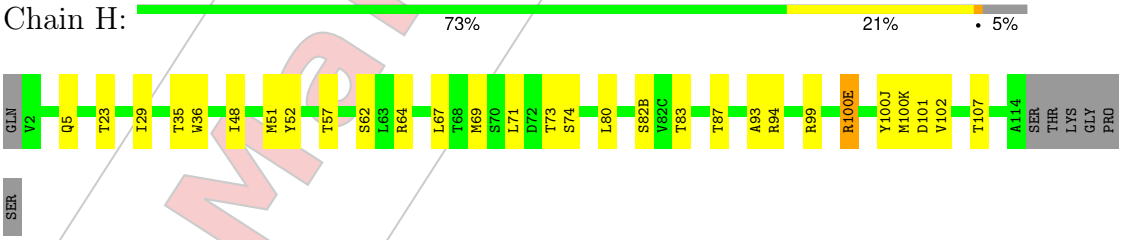
• Molecule 2: Hemagglutinin HA2

Chain F:



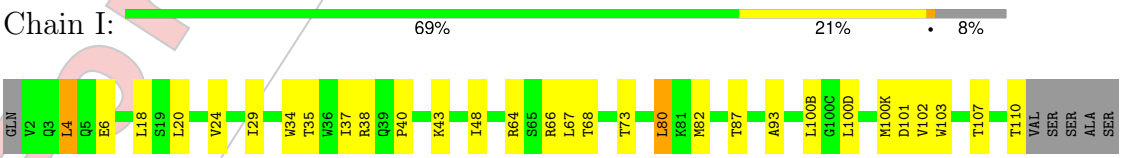
• Molecule 3: Heavy chain of Fab from human antibody 604

Chain H:



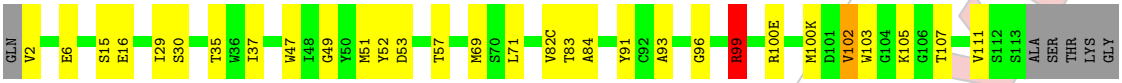
• Molecule 3: Heavy chain of Fab from human antibody 604

Chain I:



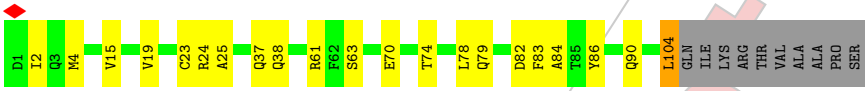
• Molecule 3: Heavy chain of Fab from human antibody 604

Chain M:



• Molecule 4: Light chain of Fab from human antibody 604

Chain J:



• Molecule 4: Light chain of Fab from human antibody 604

Chain L:

• Molecule 4: Light chain of Fab from human antibody 604

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	286029	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.706	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	380.87997, 380.87997, 380.87997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.44	0/2492	0.69	0/3403
1	C	0.42	1/2450 (0.0%)	0.65	0/3349
1	E	0.44	1/2465 (0.0%)	0.65	1/3369 (0.0%)
2	B	0.42	0/1361	0.65	0/1833
2	D	0.46	0/1357	0.68	2/1829 (0.1%)
2	F	0.42	0/1365	0.65	2/1838 (0.1%)
3	H	0.46	0/998	0.69	0/1353
3	I	0.35	0/974	0.54	0/1320
3	M	0.49	0/985	0.76	0/1337
4	J	0.22	0/815	0.42	0/1110
4	L	0.19	0/807	0.40	0/1099
4	N	0.37	0/808	0.56	0/1101
All	All	0.42	2/16877 (0.0%)	0.64	5/22941 (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
1	A	0	2
1	C	0	2
1	E	0	4
3	H	0	2
3	I	0	2
3	M	0	1
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	210	SER	C-N	-5.78	1.26	1.33
1	C	171	ASN	C-N	5.53	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	280	LYS	N-CA-C	-6.67	104.85	114.12
2	F	9	PHE	CB-CA-C	6.48	123.31	110.42
2	D	9	PHE	CA-CB-CG	6.47	120.27	113.80
2	D	9	PHE	CB-CA-C	6.18	122.72	110.42
2	F	9	PHE	CA-CB-CG	5.08	118.88	113.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	82	ARG	Sidechain
1	C	315	ARG	Sidechain
1	C	321	ARG	Sidechain
1	E	120	ARG	Sidechain
1	E	211	ARG	Sidechain
1	E	220	ARG	Sidechain
1	E	82	ARG	Sidechain
3	H	100(E)	ARG	Sidechain
3	H	64	ARG	Sidechain
3	I	64	ARG	Sidechain
3	I	66	ARG	Sidechain
3	M	99	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	2428	0	2298	35	0
1	C	2386	0	2238	39	0
1	E	2401	0	2256	38	0
2	B	1334	0	1250	22	0
2	D	1330	0	1237	31	0
2	F	1338	0	1254	26	0
3	H	977	0	961	19	0
3	I	953	0	937	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	964	0	939	26	0
4	J	796	0	756	15	0
4	L	788	0	749	16	0
4	N	790	0	749	8	0
All	All	16485	0	15624	257	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 8.

All (257) 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)
3:M:6:GLU:HB2	3:M:107:THR:CG2	1.87	1.05
3:M:6:GLU:HB2	3:M:107:THR:HG21	1.58	0.85
3:M:6:GLU:HB2	3:M:107:THR:HG23	1.57	0.83
1:A:174:LYS:HD2	1:A:261:SER:OG	1.85	0.77
1:C:82:ARG:NH2	1:C:83(A):SER:O	2.20	0.75
2:B:26:HIS:HB2	2:B:149:MET:HE3	1.67	0.74
2:D:60:ASN:OD1	2:D:60:ASN:O	2.05	0.74
1:C:283:THR:HG22	1:C:285:GLN:H	1.54	0.72
1:C:58:PRO:O	1:C:82:ARG:NH1	2.22	0.71
1:A:110:GLU:OE2	2:D:79:ASN:ND2	2.24	0.70
2:B:79:ASN:ND2	1:E:110:GLU:OE2	2.25	0.70
1:C:74:PRO:HB2	1:C:141:HIS:HB2	1.75	0.69
1:C:87:ILE:HB	1:C:267:ILE:HG12	1.73	0.69
3:M:6:GLU:CB	3:M:107:THR:HG21	2.23	0.68
3:H:101:ASP:OD1	3:H:102:VAL:N	2.28	0.66
1:C:48:ASN:HD21	1:C:287:ALA:HB3	1.58	0.66
3:I:38:ARG:HG3	3:I:48:ILE:HD11	1.78	0.66
3:H:5:GLN:NE2	3:H:23:THR:O	2.29	0.66
4:N:93:THR:HG22	4:N:95:SER:H	1.61	0.63
1:C:237:LEU:HD21	1:C:243:ILE:HB	1.80	0.63
2:B:28:ASN:HD22	2:B:149:MET:HE2	1.64	0.63
3:M:100(K):MET:HE1	4:N:98:PHE:HZ	1.62	0.62
4:J:63:SER:HG	4:J:74:THR:HG1	1.46	0.62
1:E:167:SER:HB3	1:E:244:ILE:HG12	1.82	0.61
2:D:58:LYS:HB3	2:F:94:TYR:CE1	2.36	0.61
3:M:51:MET:HG3	3:M:57:THR:HG22	1.82	0.61
1:E:39:SER:HB2	1:E:315:ARG:HH11	1.66	0.61
2:D:26:HIS:HB2	2:D:149:MET:HE3	1.82	0.60
4:J:83:PHE:CD1	4:J:104:LEU:HD22	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:4:MET:HE3	4:L:25:ALA:HB2	1.83	0.60
3:M:2:VAL:HG13	3:M:102:VAL:HG11	1.83	0.60
2:D:98:LEU:O	2:D:102:LEU:HG	2.02	0.60
3:H:67:LEU:HD22	3:H:80:LEU:HD11	1.83	0.59
1:E:26:VAL:HG11	1:E:317:VAL:HG22	1.85	0.59
2:D:14:TRP:HE3	2:D:17:MET:HE2	1.68	0.59
3:M:37:ILE:HD12	3:M:103:TRP:CH2	2.39	0.58
4:L:31:SER:O	4:L:31:SER:OG	2.21	0.58
4:J:4:MET:HE3	4:J:25:ALA:HB2	1.85	0.57
3:M:29:ILE:HG21	3:M:71:LEU:HD22	1.87	0.57
1:A:295:GLN:HG2	1:A:306:PRO:HG2	1.86	0.57
1:E:191:GLN:HE22	1:E:250:ASN:HD21	1.53	0.56
3:I:100(B):LEU:HB3	3:I:100(D):LEU:HD13	1.88	0.56
4:L:5:THR:HA	4:L:100:GLN:HE22	1.71	0.56
3:H:99:ARG:HH11	3:H:100(J):TYR:HE1	1.54	0.56
3:I:67:LEU:HD22	3:I:80:LEU:HD11	1.88	0.55
2:B:123:LYS:HD2	2:B:132:GLU:OE2	2.07	0.55
3:M:83:THR:HG22	3:M:84:ALA:N	2.21	0.55
2:F:9:PHE:HZ	2:F:119:TYR:CG	2.24	0.54
3:H:94:ARG:O	3:H:101:ASP:OD1	2.25	0.54
3:H:51:MET:HG2	3:H:71:LEU:HD12	1.89	0.54
2:D:75:ARG:NH1	2:D:78:GLU:OE1	2.41	0.54
1:E:15:ILE:HD13	2:F:119:TYR:HA	1.90	0.54
1:E:250:ASN:OD1	1:E:250:ASN:N	2.39	0.54
4:L:7:SER:HB2	4:L:8:PRO:HD3	1.90	0.54
4:J:79:GLN:N	4:J:79:GLN:OE1	2.41	0.53
2:B:148:CYS:O	2:B:152:VAL:HG23	2.08	0.53
2:B:98:LEU:O	2:B:102:LEU:HG	2.08	0.53
1:C:28:THR:HG22	1:C:30:LEU:H	1.74	0.53
2:B:76:ARG:NH1	1:E:107:GLU:OE1	2.33	0.53
1:C:15:ILE:HD13	2:D:119:TYR:HA	1.92	0.52
1:A:138:SER:HB3	1:A:224:ARG:HG2	1.91	0.52
4:J:84:ALA:H	4:J:104:LEU:CD1	2.21	0.52
1:A:62:GLY:H	1:A:79:LEU:HD11	1.74	0.52
1:E:221:PRO:O	1:E:229:ARG:NH2	2.42	0.52
2:F:99:LEU:HD12	2:F:103:GLU:HG3	1.91	0.52
4:J:24:ARG:HG2	4:J:70:GLU:HG2	1.91	0.52
1:C:139:CYS:O	1:C:146:SER:OG	2.26	0.52
1:E:200:ALA:HB1	1:E:249:GLY:HA3	1.93	0.51
3:H:100(K):MET:HE1	4:L:98:PHE:HZ	1.75	0.51
2:D:9:PHE:HZ	2:D:119:TYR:CG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:ILE:HD11	2:F:139:GLU:HB2	1.92	0.51
2:D:54:SER:O	2:D:58:LYS:HB2	2.11	0.51
3:M:35:THR:HG23	3:M:93:ALA:HB3	1.92	0.51
3:M:83:THR:HG22	3:M:84:ALA:H	1.75	0.51
1:C:307:LYS:NZ	2:D:61:THR:HG22	2.25	0.51
1:A:48:ASN:HD21	1:A:287:ALA:HB3	1.76	0.51
1:E:11:ASP:N	2:F:27:GLN:O	2.44	0.51
4:L:61:ARG:NE	4:L:82:ASP:OD2	2.43	0.51
1:E:318:THR:HG23	2:F:48:ILE:HG21	1.92	0.51
3:I:87:THR:HB	3:I:110:THR:HA	1.92	0.51
2:B:94:TYR:CE1	2:F:58:LYS:HB3	2.46	0.51
1:C:206:SER:HB3	1:C:243:ILE:HD13	1.93	0.51
4:L:89:GLN:NE2	4:L:96:SER:OG	2.28	0.51
3:M:91:TYR:HD1	3:M:105:LYS:O	1.94	0.50
4:N:81:ASP:C	4:N:83:PHE:H	2.19	0.50
1:C:211:ARG:HG2	1:C:213:PHE:CZ	2.46	0.50
2:B:161:LYS:NZ	2:B:161:LYS:HB3	2.27	0.50
3:H:82(B):SER:O	3:H:82(B):SER:OG	2.29	0.50
1:C:197:LYS:NZ	1:C:248:ASN:HB2	2.26	0.50
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.94	0.49
1:E:59:LEU:HB2	1:E:82:ARG:HD2	1.92	0.49
1:A:161:TYR:CE2	1:A:249:GLY:HA2	2.47	0.49
3:H:101:ASP:OD1	3:H:102:VAL:HG23	2.12	0.49
3:M:15:SER:O	3:M:15:SER:OG	2.31	0.49
1:A:318:THR:HG23	2:B:48:ILE:HG21	1.93	0.49
3:H:35:THR:HG23	3:H:93:ALA:HB3	1.95	0.49
1:A:127:TRP:HZ3	1:A:164:LEU:HD11	1.77	0.49
2:F:119:TYR:OH	2:F:132:GLU:OE2	2.21	0.49
3:I:4:LEU:HD23	3:I:24:VAL:HG22	1.95	0.49
4:L:63:SER:OG	4:L:74:THR:OG1	2.28	0.49
1:A:164:LEU:HB3	1:A:247:ALA:O	2.12	0.48
2:D:85:ASP:OD1	2:F:83:LYS:NZ	2.37	0.48
1:E:51:LEU:HB2	1:E:274:MET:HA	1.95	0.48
3:M:91:TYR:CD1	3:M:105:LYS:O	2.65	0.48
1:A:61:LEU:HD21	1:A:69:TRP:HB2	1.93	0.48
3:M:84:ALA:HA	3:M:111:VAL:HB	1.94	0.48
1:E:125:PRO:O	1:E:126:SER:HB3	2.12	0.48
1:E:132:THR:HB	1:E:152:LEU:HD21	1.95	0.48
1:C:216:GLU:OE2	1:C:220:ARG:NH2	2.47	0.48
3:I:35:THR:HG23	3:I:93:ALA:HB3	1.96	0.48
3:H:29:ILE:HG21	3:H:71:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:PRO:HG2	1:C:217:ILE:HD12	1.95	0.48
1:C:204:VAL:HG12	1:C:243:ILE:HD11	1.96	0.47
2:D:131:LYS:HB3	2:D:139:GLU:HB3	1.96	0.47
3:I:29:ILE:HG21	3:I:73:THR:HA	1.97	0.47
3:I:40:PRO:HB2	3:I:43:LYS:HG3	1.95	0.47
1:C:125(A):LYS:HB2	1:C:255:ARG:HD2	1.95	0.47
3:I:18:LEU:HD23	3:I:82:MET:HE2	1.97	0.47
1:C:127:TRP:HZ3	1:C:164:LEU:HD13	1.79	0.47
2:F:98:LEU:O	2:F:102:LEU:HG	2.14	0.47
3:M:82(C):VAL:HG12	3:M:111:VAL:HG11	1.96	0.47
2:B:58:LYS:HE3	2:D:97:GLU:HB3	1.97	0.47
1:E:310:ARG:NH2	2:F:90:ASP:OD1	2.35	0.47
4:L:90:GLN:HE21	4:L:97:THR:H	1.63	0.47
2:D:77:MET:HE2	2:D:77:MET:HB2	1.88	0.47
1:E:262:ARG:HD2	1:E:262:ARG:N	2.30	0.47
2:F:135:ASN:O	2:F:135:ASN:ND2	2.48	0.46
3:H:52:TYR:HB3	3:H:100(E):ARG:HH21	1.78	0.46
1:A:18:HIS:ND1	2:B:17:MET:O	2.46	0.46
1:E:69:TRP:HH2	1:E:84:TRP:CH2	2.33	0.46
3:I:4:LEU:HD21	3:I:34:TRP:HZ3	1.81	0.46
4:N:4:MET:HE3	4:N:90:GLN:HB3	1.98	0.46
1:C:99:PRO:HB2	1:C:229:ARG:HD3	1.98	0.46
2:D:162:TYR:O	2:D:166:SER:OG	2.32	0.46
1:E:126:SER:OG	1:E:166:LYS:HE2	2.16	0.46
1:A:54:LEU:HD21	2:B:63:PHE:HE2	1.80	0.46
2:F:123:LYS:HB3	2:F:123:LYS:HE2	1.44	0.46
3:I:29:ILE:HA	3:I:34:TRP:HZ2	1.81	0.46
4:J:86:TYR:HE2	4:J:104:LEU:CD1	2.29	0.45
2:D:91:ILE:HG21	2:F:91:ILE:HD13	1.98	0.45
2:D:99:LEU:HD13	2:F:98:LEU:HD13	1.98	0.45
2:D:160:PRO:HA	2:D:163:SER:HB3	1.97	0.45
1:A:151:LEU:HB3	1:A:252:ILE:HG22	1.98	0.45
1:A:174:LYS:HD2	1:A:261:SER:HG	1.79	0.45
2:B:133:ILE:HG21	2:B:139:GLU:HB2	1.99	0.45
4:J:19:VAL:HG21	4:J:78:LEU:HD11	1.98	0.45
1:C:133(A):THR:O	1:C:133(A):THR:OG1	2.35	0.45
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.99	0.45
4:J:83:PHE:HD1	4:J:104:LEU:HD22	1.79	0.45
2:B:17:MET:HE3	2:B:17:MET:HB2	1.59	0.44
1:C:132:THR:HB	1:C:152:LEU:HD11	1.99	0.44
2:D:66:VAL:HG12	2:D:66:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:HB2	1:A:141:HIS:HB2	2.00	0.44
1:E:229:ARG:HA	1:E:229:ARG:HD3	1.71	0.44
4:N:7:SER:HB2	4:N:8:PRO:HD2	1.97	0.44
1:C:20:ASN:O	1:C:322:ASN:ND2	2.48	0.44
1:C:282:GLN:HB3	1:C:302:ILE:HG23	1.99	0.44
2:F:58:LYS:HD3	2:F:58:LYS:HA	1.63	0.44
4:J:61:ARG:NE	4:J:82:ASP:OD2	2.49	0.44
1:A:15:ILE:HD13	2:B:119:TYR:HA	2.00	0.44
2:D:59:MET:HE2	2:D:59:MET:HB2	1.77	0.44
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.53	0.44
3:M:52:TYR:CD1	3:M:100(E):ARG:HG3	2.52	0.44
1:C:307:LYS:HZ1	2:D:61:THR:HG22	1.82	0.44
2:D:118:LEU:HD12	2:D:118:LEU:HA	1.89	0.44
1:E:25:THR:HG23	1:E:33:ASN:HA	2.00	0.43
3:H:36:TRP:CD1	3:H:69:MET:HE2	2.53	0.43
3:M:16:GLU:O	3:M:82(C):VAL:HG23	2.18	0.43
1:E:43:LEU:HD13	1:E:314:LEU:HD12	1.99	0.43
1:E:82:ARG:HD3	1:E:84:TRP:HE3	1.83	0.43
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.53	0.43
2:D:9:PHE:HE2	2:D:136:GLY:HA2	1.83	0.43
3:H:48:ILE:HG22	3:H:69:MET:HE3	2.00	0.43
2:B:77:MET:HE1	2:F:77:MET:SD	2.58	0.43
1:A:19:ALA:O	2:B:15:THR:HA	2.19	0.43
2:B:50:ASN:OD1	1:C:32:LYS:NZ	2.51	0.43
2:D:58:LYS:HB3	2:F:94:TYR:HE1	1.82	0.43
3:I:37:ILE:HD12	3:I:103:TRP:CH2	2.53	0.43
2:F:120:GLU:OE1	2:F:120:GLU:HA	2.19	0.43
3:H:73:THR:O	3:H:74:SER:C	2.61	0.43
1:A:149:LYS:HE3	1:A:149:LYS:HB3	1.82	0.43
1:A:157:LYS:HG3	1:A:158:ASN:OD1	2.19	0.43
2:D:58:LYS:HA	2:D:58:LYS:HD3	1.61	0.43
4:J:82:ASP:O	4:J:104:LEU:HD11	2.19	0.43
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.90	0.43
1:A:133(A):THR:O	1:A:133(A):THR:OG1	2.36	0.43
3:M:100(K):MET:HE3	3:M:100(K):MET:HB2	1.87	0.43
1:E:122:GLU:HG3	1:E:255:ARG:O	2.19	0.43
1:E:301:THR:HB	1:E:305:CYS:SG	2.59	0.43
4:L:6:GLN:NE2	4:L:35:TRP:HZ3	2.17	0.43
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.86	0.42
1:E:89:GLU:O	1:E:269:ASN:HA	2.19	0.42
2:F:54:SER:O	2:F:58:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:30:SER:HA	3:M:53:ASP:OD2	2.19	0.42
1:C:125(A):LYS:HE3	1:C:132:THR:OG1	2.19	0.42
1:E:183:HIS:HB3	1:E:250:ASN:HB3	2.01	0.42
1:E:317:VAL:HG23	2:F:104:ASN:CG	2.44	0.42
4:J:4:MET:HE2	4:J:23:CYS:SG	2.59	0.42
4:L:11:LEU:HD23	4:L:19:VAL:HG13	2.01	0.42
3:M:47:TRP:CZ2	3:M:49:GLY:HA2	2.54	0.42
2:B:49:THR:HG21	4:L:32:TRP:HZ2	1.85	0.42
1:C:122:GLU:HG2	1:C:256:TYR:HE1	1.83	0.42
4:J:15:VAL:HG13	4:J:78:LEU:O	2.20	0.42
1:A:262:ARG:HA	1:A:262:ARG:HD3	1.72	0.42
2:F:168:LEU:HD23	2:F:168:LEU:HA	1.82	0.42
3:M:93:ALA:HB1	3:M:100(K):MET:HB3	2.02	0.42
1:E:74:PRO:HB2	1:E:141:HIS:HB2	2.01	0.42
2:F:101:LEU:HD23	2:F:101:LEU:HA	1.92	0.42
1:A:89:GLU:O	1:A:269:ASN:HA	2.20	0.42
1:A:155:THR:HG22	1:A:156:GLY:N	2.35	0.42
1:E:164:LEU:HD11	1:E:251:LEU:HD23	2.02	0.42
3:M:49:GLY:HA3	3:M:69:MET:HE1	2.02	0.42
1:A:61:LEU:HA	1:A:79:LEU:HD13	2.02	0.42
1:C:70:ILE:HD12	1:C:70:ILE:HA	1.93	0.42
1:A:99:PRO:HB2	1:A:229:ARG:HD3	2.02	0.42
1:E:100:GLY:HA3	1:E:230:ILE:O	2.20	0.42
4:L:19:VAL:HG11	4:L:104:LEU:HD11	2.01	0.42
2:D:97:GLU:O	2:D:101:LEU:HD13	2.20	0.41
2:F:134:GLY:C	2:F:136:GLY:H	2.28	0.41
1:C:262:ARG:HA	1:C:262:ARG:HD3	1.77	0.41
2:D:25:HIS:NE2	2:D:32:SER:OG	2.53	0.41
3:I:37:ILE:HD11	3:I:100(K):MET:SD	2.60	0.41
4:J:38:GLN:O	4:J:84:ALA:HB1	2.20	0.41
3:M:96:GLY:HA3	3:M:99:ARG:HG3	2.00	0.41
1:C:19:ALA:O	2:D:15:THR:HA	2.21	0.41
1:A:174:LYS:CD	1:A:261:SER:OG	2.63	0.41
1:C:316:MET:HE2	1:C:316:MET:HB3	1.73	0.41
1:E:237:LEU:HD23	1:E:237:LEU:HA	1.84	0.41
2:B:30:GLN:NE2	2:B:145:ASN:HB2	2.35	0.41
3:H:100(K):MET:HE1	4:L:98:PHE:CZ	2.54	0.41
3:I:101:ASP:OD1	3:I:102:VAL:HG23	2.20	0.41
4:N:81:ASP:C	4:N:83:PHE:N	2.79	0.41
1:E:97:CYS:SG	1:E:98:TYR:N	2.94	0.41
4:L:61:ARG:HB2	4:L:76:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ALA:HA	1:A:242:THR:HG22	2.02	0.41
1:E:196:HIS:C	1:E:197:LYS:HG2	2.46	0.41
3:I:6:GLU:HB2	3:I:107:THR:HG23	2.03	0.41
4:N:2:ILE:HB	4:N:90:GLN:NE2	2.35	0.41
4:N:78:LEU:HD23	4:N:78:LEU:HA	1.82	0.41
1:A:111:GLN:OE1	1:A:262:ARG:NH2	2.50	0.41
1:A:303:GLY:HA2	2:B:63:PHE:CE2	2.55	0.41
1:C:25:THR:HG23	1:C:33:ASN:HA	2.02	0.41
3:H:35:THR:HG21	3:H:100(K):MET:HG2	2.03	0.41
1:E:266:GLY:HA3	1:E:302:ILE:HD11	2.02	0.40
1:E:295:GLN:HG2	1:E:306:PRO:HG2	2.03	0.40
2:F:59:MET:HE2	2:F:59:MET:HB2	1.93	0.40
1:A:110:GLU:HG3	2:D:76:ARG:HG2	2.03	0.40
1:C:238:GLU:H	1:C:238:GLU:HG3	1.66	0.40
3:H:100(K):MET:HE3	3:H:100(K):MET:HB2	1.71	0.40
3:M:49:GLY:C	3:M:69:MET:HE1	2.46	0.40
1:C:307:LYS:NZ	2:D:61:THR:CG2	2.85	0.40
4:L:38:GLN:O	4:L:84:ALA:HB1	2.21	0.40
1:C:191:GLN:HE21	1:C:198:GLU:HA	1.86	0.40
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.56	0.40
1:A:197:LYS:HD2	1:A:248:ASN:O	2.21	0.40
3:H:29:ILE:CG2	3:H:71:LEU:HD22	2.52	0.40
4:J:2:ILE:HB	4:J:90:GLN:NE2	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	317/326 (97%)	296 (93%)	20 (6%)	1 (0%)	37 60
1	C	315/326 (97%)	293 (93%)	20 (6%)	2 (1%)	22 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	316/326 (97%)	291 (92%)	24 (8%)	1 (0%)	37	60
2	B	167/222 (75%)	161 (96%)	6 (4%)	0	100	100
2	D	167/222 (75%)	162 (97%)	5 (3%)	0	100	100
2	F	167/222 (75%)	157 (94%)	10 (6%)	0	100	100
3	H	125/134 (93%)	118 (94%)	7 (6%)	0	100	100
3	I	121/134 (90%)	118 (98%)	3 (2%)	0	100	100
3	M	124/134 (92%)	116 (94%)	8 (6%)	0	100	100
4	J	102/114 (90%)	97 (95%)	5 (5%)	0	100	100
4	L	101/114 (89%)	94 (93%)	7 (7%)	0	100	100
4	N	102/114 (90%)	94 (92%)	8 (8%)	0	100	100
All	All	2124/2388 (89%)	1997 (94%)	123 (6%)	4 (0%)	45	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	119	GLU
1	C	197	LYS
1	E	290	SER
1	A	82	ARG

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	256/286 (90%)	248 (97%)	8 (3%)	35	63
1	C	246/286 (86%)	231 (94%)	15 (6%)	15	35
1	E	250/286 (87%)	243 (97%)	7 (3%)	38	66
2	B	138/191 (72%)	136 (99%)	2 (1%)	62	83
2	D	137/191 (72%)	131 (96%)	6 (4%)	24	49
2	F	139/191 (73%)	130 (94%)	9 (6%)	14	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	108/114 (95%)	103 (95%)	5 (5%)	23	47
3	I	105/114 (92%)	101 (96%)	4 (4%)	28	55
3	M	106/114 (93%)	104 (98%)	2 (2%)	52	77
4	J	90/98 (92%)	88 (98%)	2 (2%)	47	74
4	L	89/98 (91%)	87 (98%)	2 (2%)	47	74
4	N	89/98 (91%)	86 (97%)	3 (3%)	32	59
All	All	1753/2067 (85%)	1688 (96%)	65 (4%)	31	56

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	106	GLU
1	A	174	LYS
1	A	188	ILE
1	A	197	LYS
1	A	203	SER
1	A	224	ARG
1	A	284	PRO
2	B	15	THR
2	B	98	LEU
1	C	25	THR
1	C	106	GLU
1	C	118	PHE
1	C	119	GLU
1	C	123	ILE
1	C	164	LEU
1	C	191	GLN
1	C	197	LYS
1	C	216	GLU
1	C	242	THR
1	C	291	SER
1	C	316	MET
1	C	317	VAL
1	C	318	THR
1	C	321	ARG
2	D	9	PHE
2	D	57	GLU
2	D	58	LYS
2	D	68	LYS

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Mol	Chain	Res	Type
2	D	71	ASN
2	D	139	GLU
1	E	35	THR
1	E	82	ARG
1	E	115	VAL
1	E	152	LEU
1	E	155	THR
1	E	197	LYS
1	E	250	ASN
2	F	9	PHE
2	F	10	ILE
2	F	11	GLU
2	F	15	THR
2	F	57	GLU
2	F	58	LYS
2	F	118	LEU
2	F	123	LYS
2	F	124	SER
3	H	57	THR
3	H	62	SER
3	H	83	THR
3	H	87	THR
3	H	107	THR
3	I	4	LEU
3	I	20	LEU
3	I	68	THR
3	I	80	LEU
4	J	37	GLN
4	J	104	LEU
4	L	67	SER
4	L	79	GLN
3	M	99	ARG
3	M	102	VAL
4	N	22	THR
4	N	38	GLN
4	N	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
2	B	30	GLN

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Mol	Chain	Res	Type
2	B	169	ASN
1	C	73	ASN
1	C	92	ASN
1	C	101	HIS
1	C	282	GLN
2	D	60	ASN
2	D	129	ASN
1	E	191	GLN
1	E	196	HIS
2	F	125	GLN
2	F	135	ASN
4	J	50	GLN
4	J	90	GLN
4	L	37	GLN
4	L	90	GLN
4	L	92	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

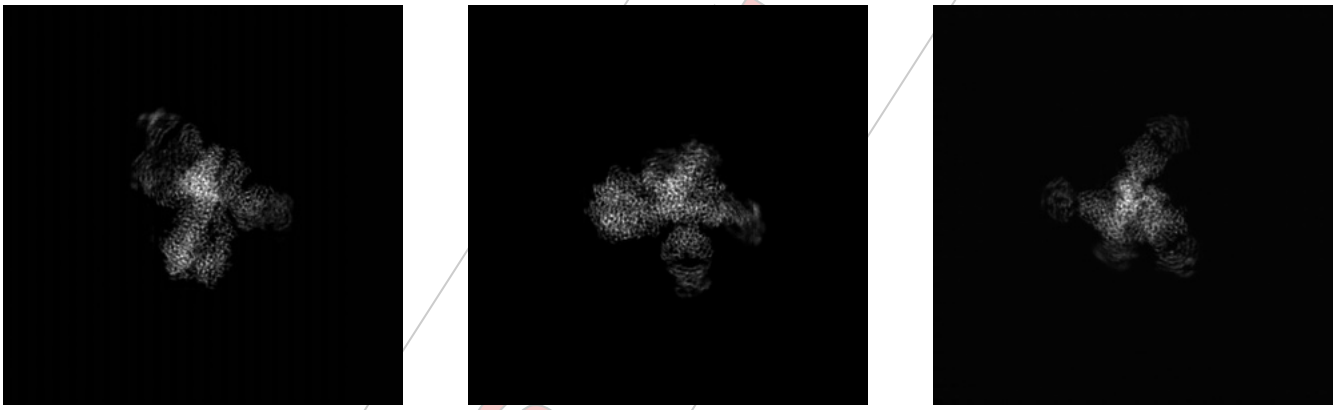
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70503. 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.

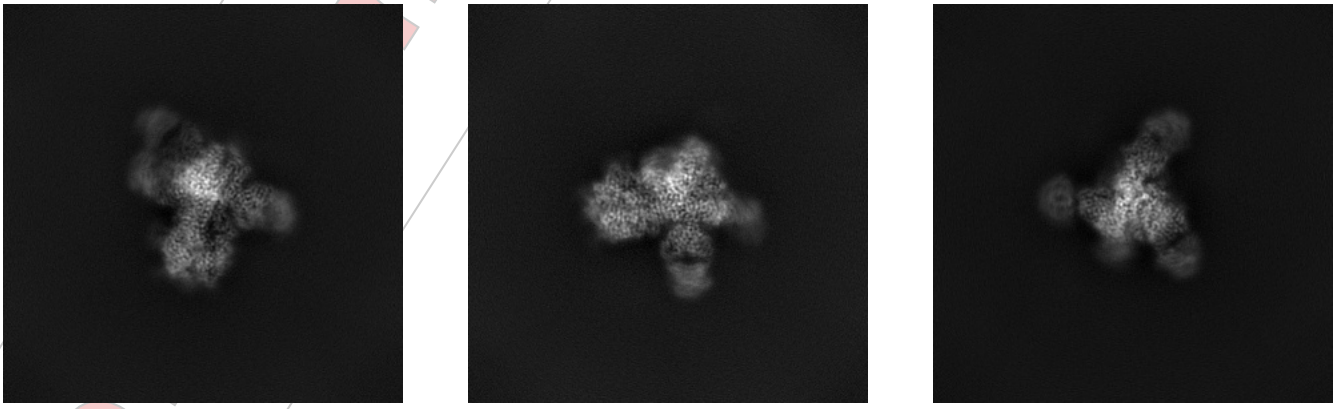
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

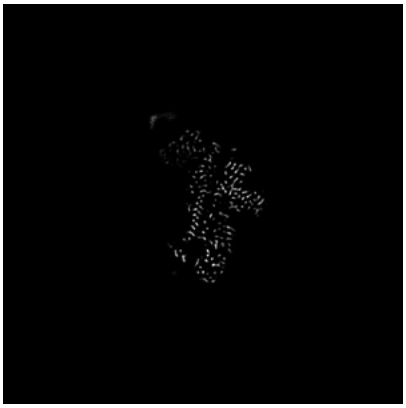


X Y Z

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

6.2 Central slices (i)

6.2.1 Primary map

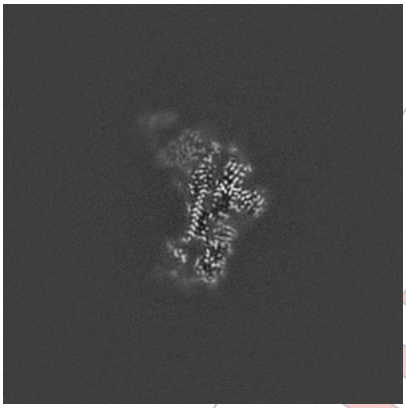


X Index: 180

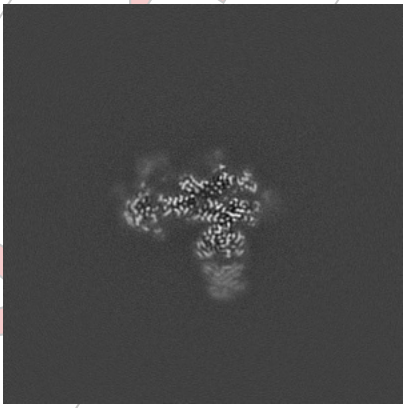
Y Index: 180

Z Index: 180

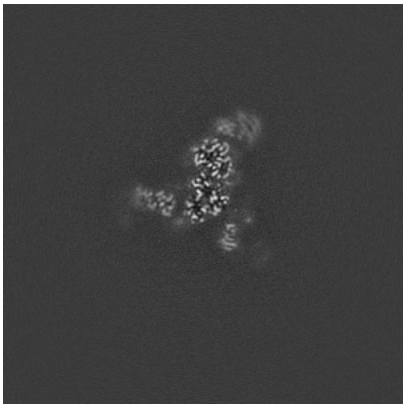
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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

6.3 Largest variance slices (i)

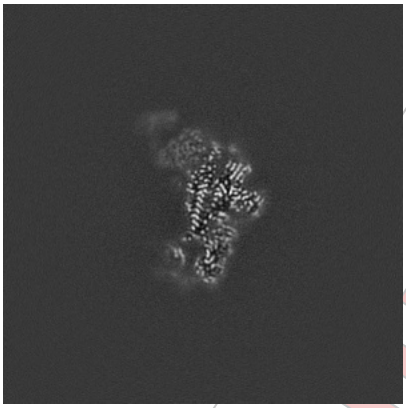
6.3.1 Primary map

X Index: 174

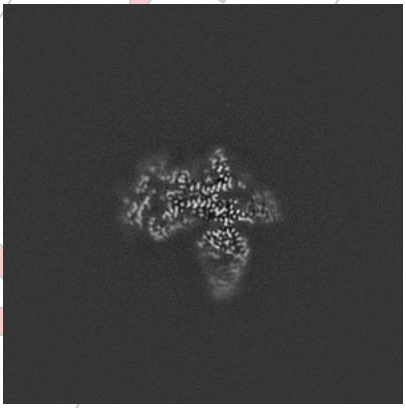
Y Index: 175

Z Index: 191

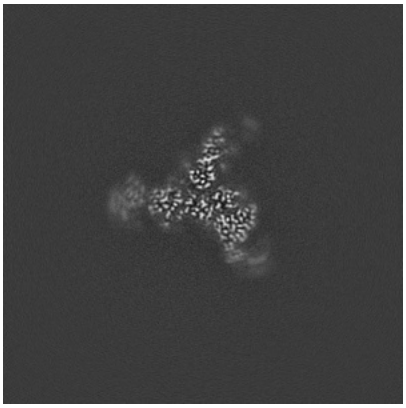
6.3.2 Raw map



X Index: 179



Y Index: 175

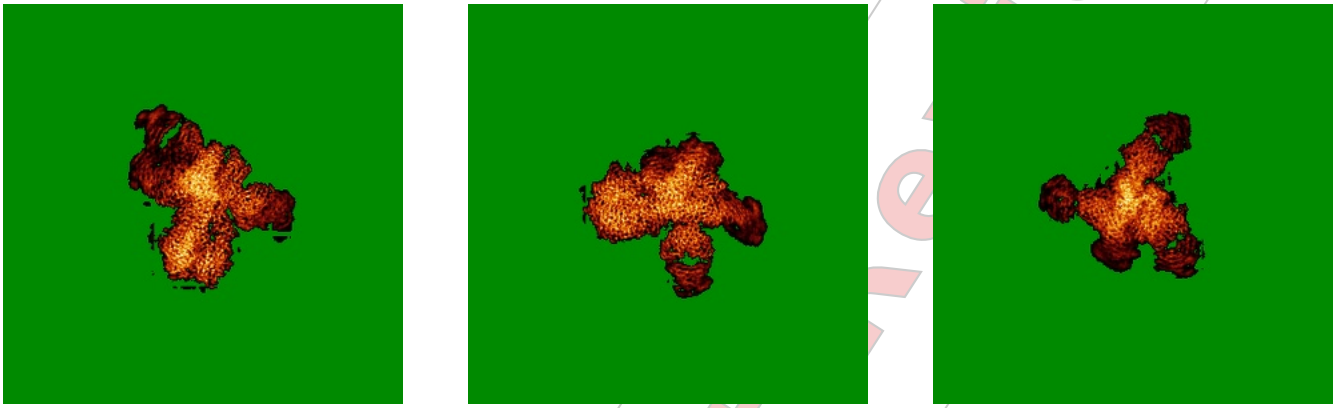


Z Index: 191

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

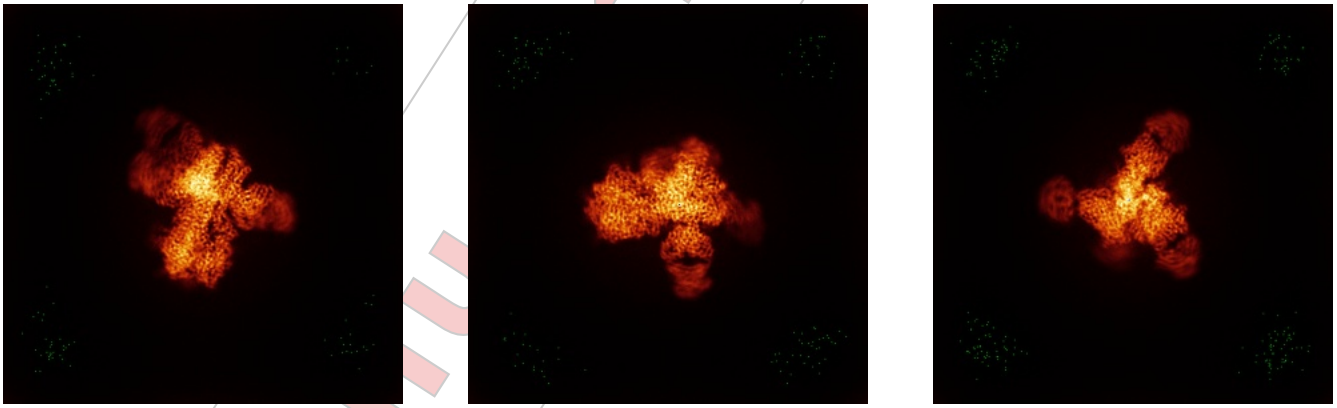
6.4 Orthogonal standard-deviation projections (False-color)

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.

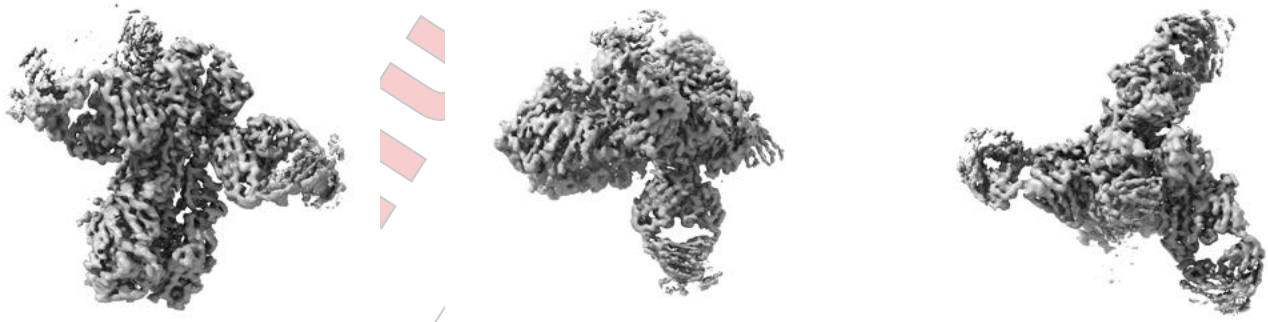
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

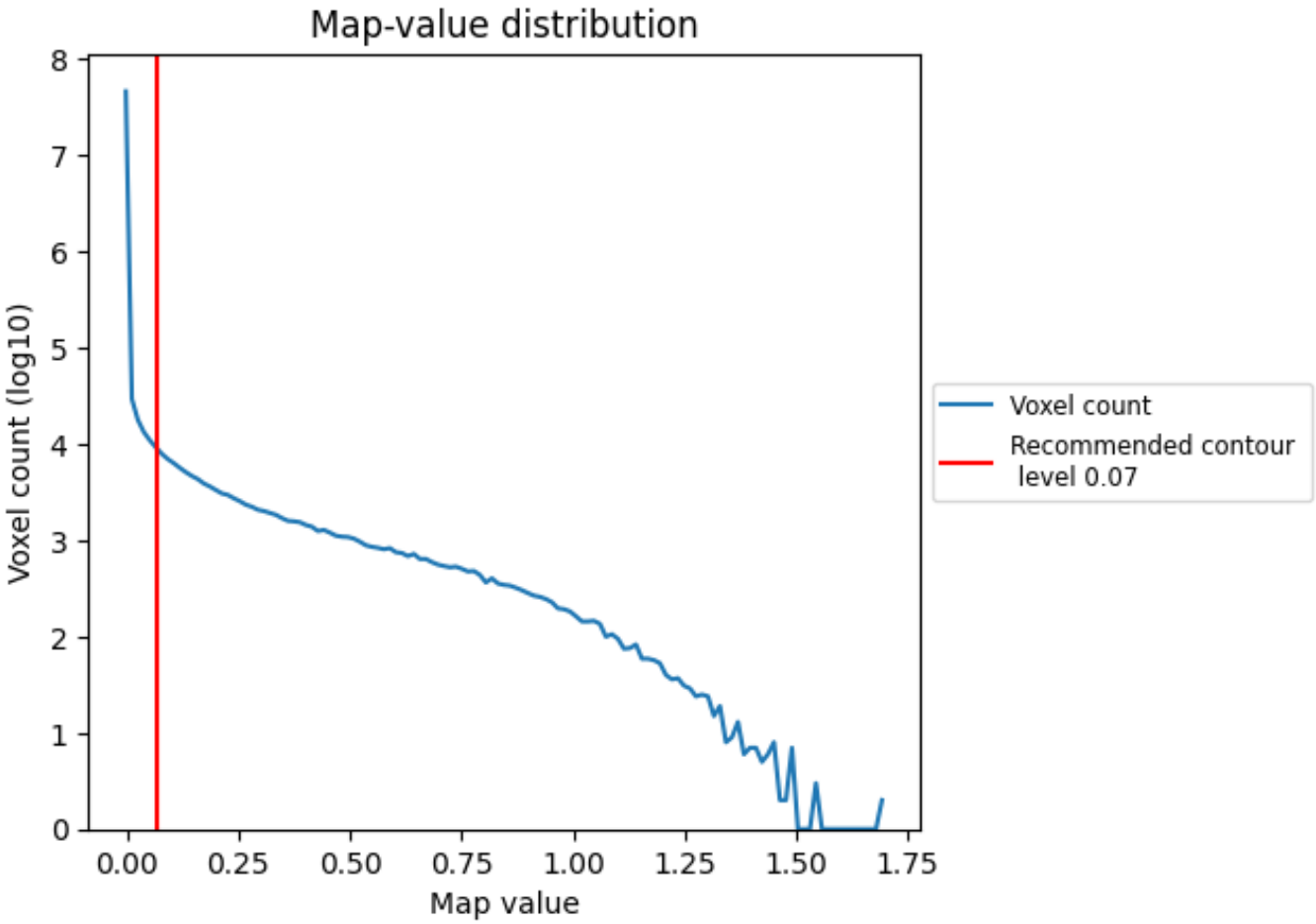
6.6 Mask visualisation (i)

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

7 Map analysis

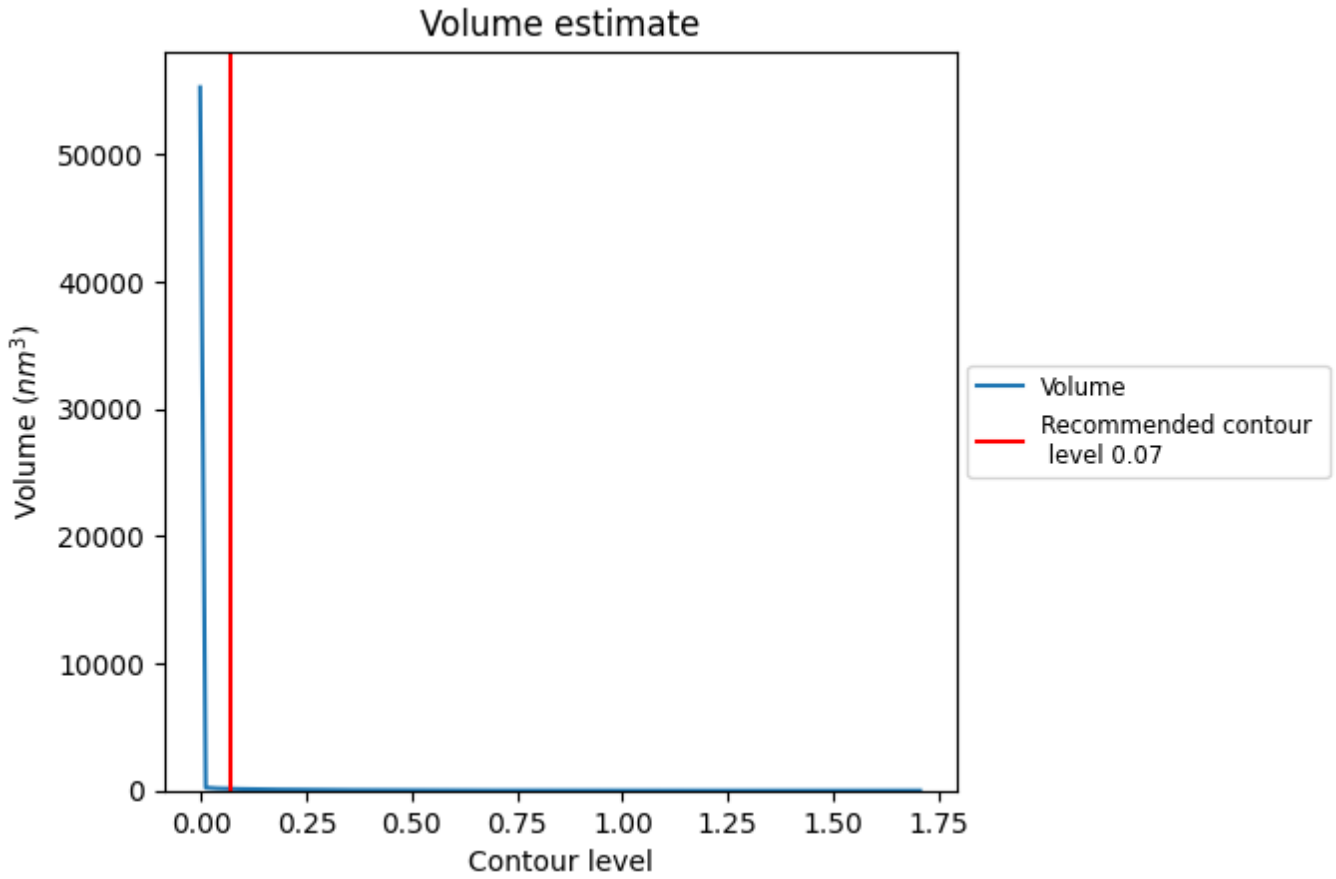
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

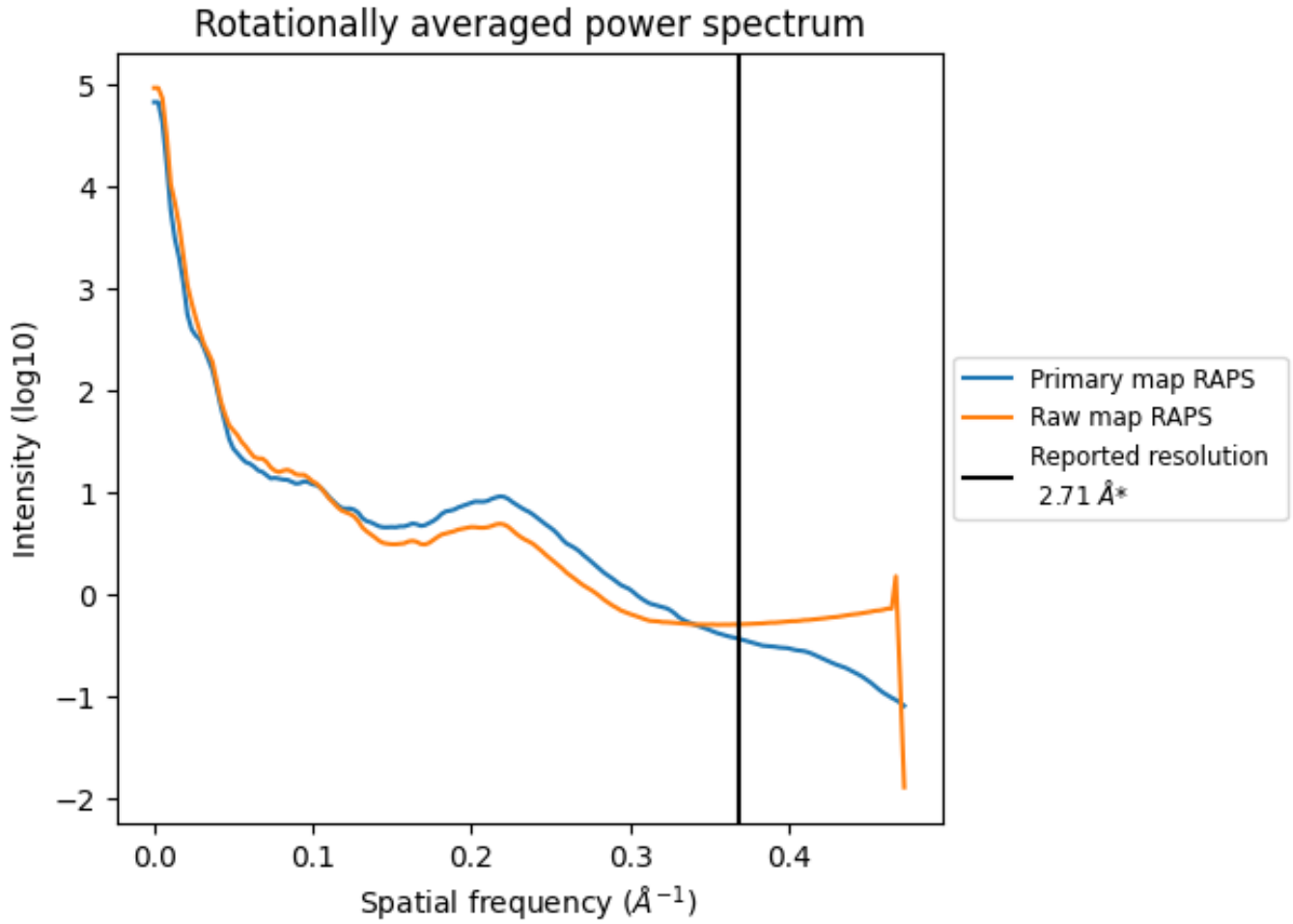
7.2 Volume estimate (i)



The volume at the recommended contour level is 141 nm^3; this corresponds to an approximate mass of 128 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)

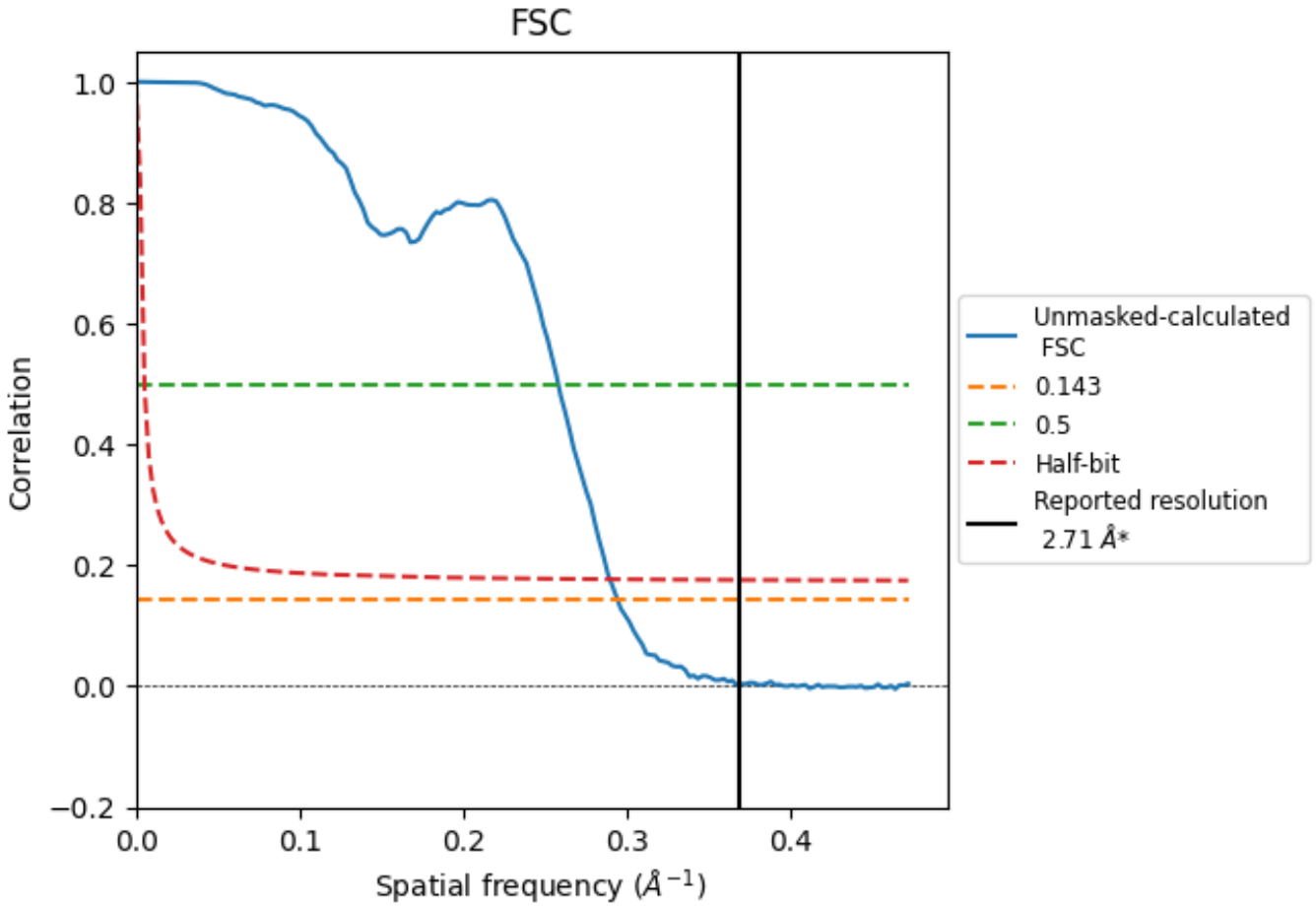


*Reported resolution corresponds to spatial frequency of 0.369 Å^{-1}

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 0.369 Å^{-1}

8.2 Resolution estimates (i)

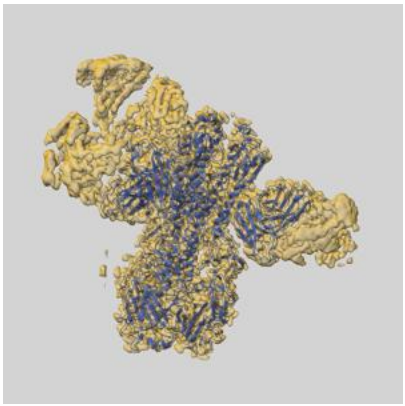
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	3.87	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 2.71 by more than 10 %

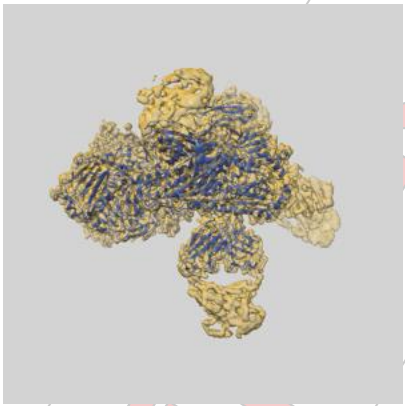
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70503 and PDB model 9OI3. Per-residue inclusion information can be found in section 3 on page 6.

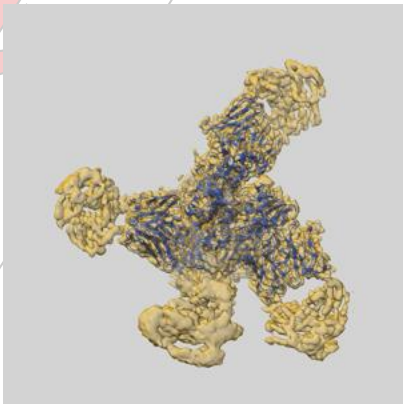
9.1 Map-model overlay



X



Y



Z

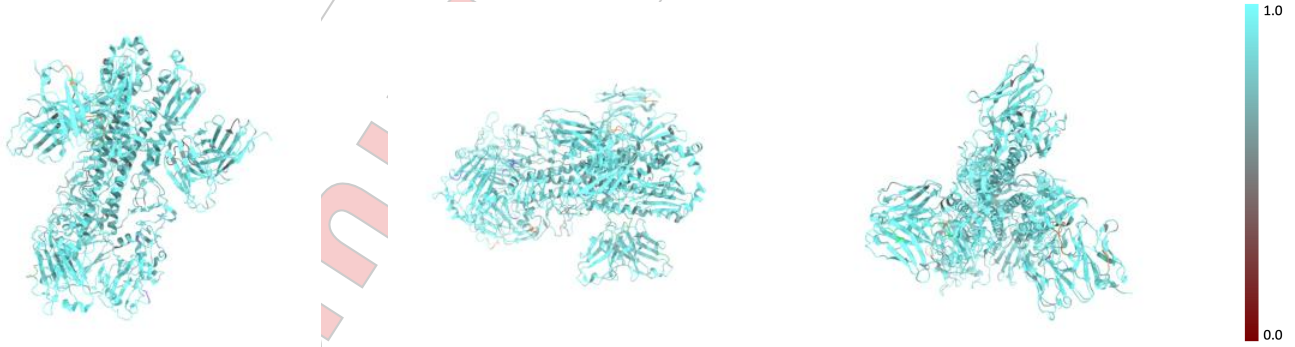
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

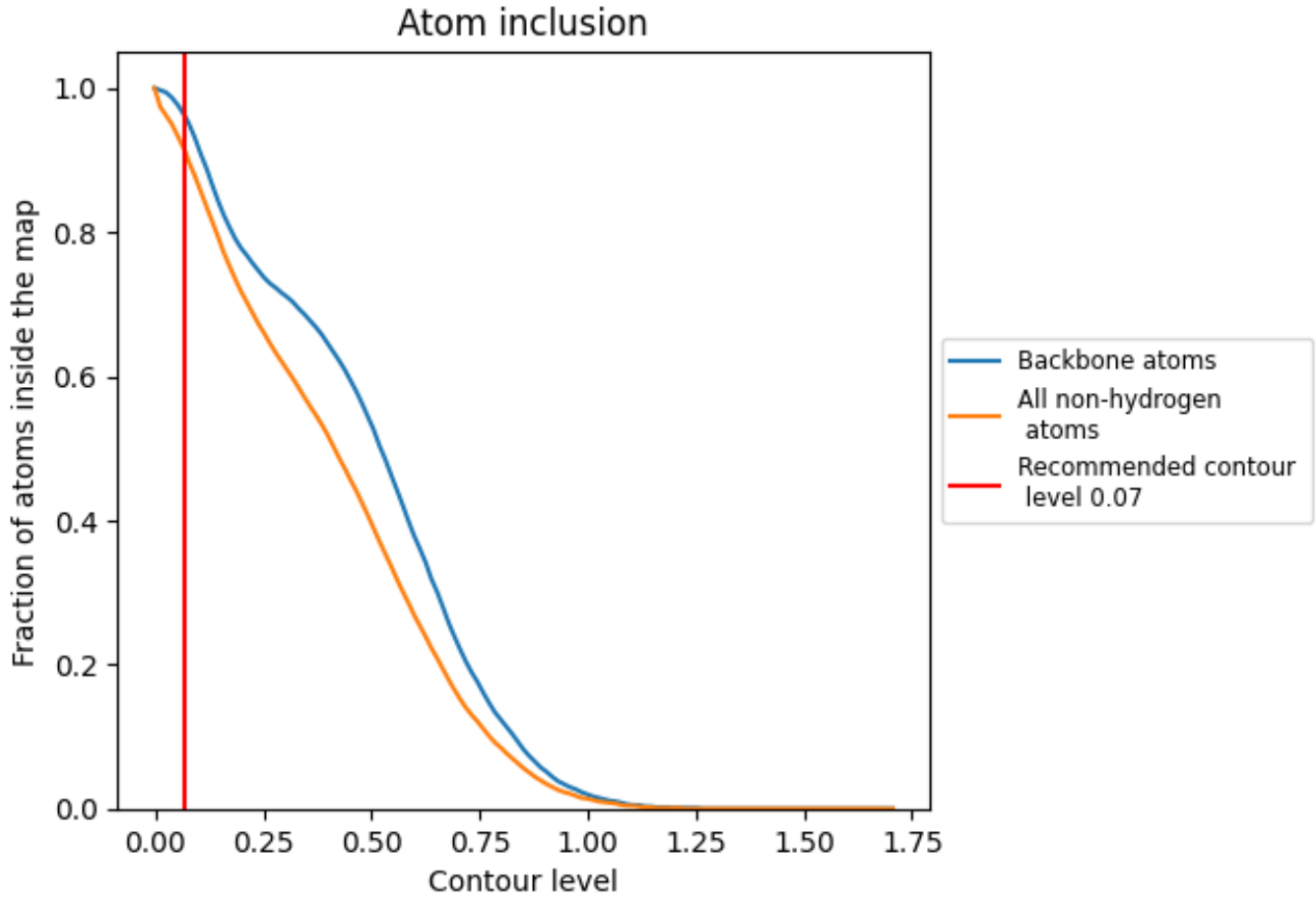
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.5570
A	0.9300	0.5630
B	0.8990	0.5630
C	0.9240	0.5540
D	0.8950	0.5620
E	0.9190	0.5550
F	0.8990	0.5630
H	0.9050	0.5530
I	0.9080	0.5620
J	0.8940	0.5400
L	0.8900	0.5470
M	0.9150	0.5670
N	0.8870	0.5380