



## wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 08:11 AM EST

PDB ID : 6DZM  
EMDB ID : EMD-8936  
Title : Bundibugyo virus GP (mucin-deleted) in complex with pan-ebolavirus human antibody ADI-15878 Fab  
Authors : Murin, C.D.; Ward, A.B.  
Deposited on : 2018-07-05  
Resolution : 4.29 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

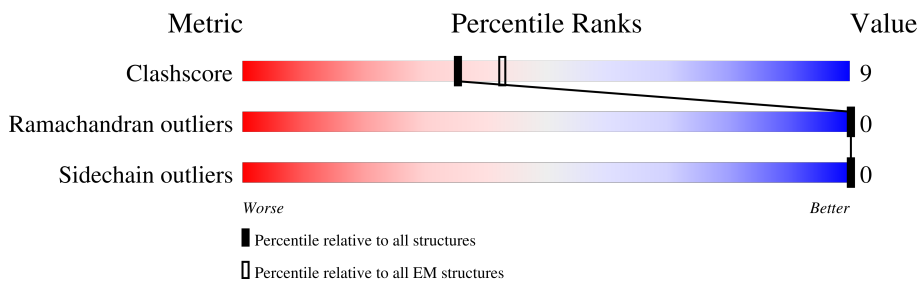
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.29 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.




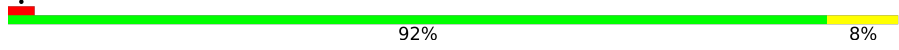
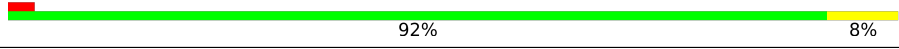
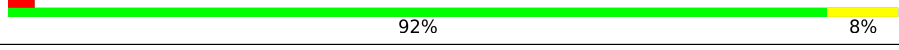



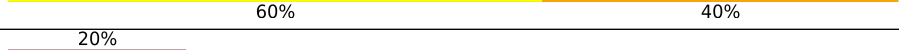
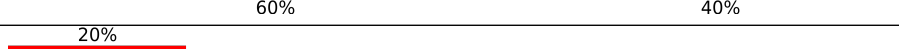
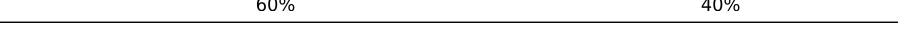
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	311	5% 61% 11% 28%
1	B	311	5% 61% 11% 28%
1	C	311	5% 61% 11% 28%
2	D	177	14% 49% 16% 35%
2	E	177	14% 49% 16% 35%
2	F	177	13% 49% 16% 35%
3	H	106	81% 19%
3	K	106	83% 17%

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Mol	Chain	Length	Quality of chain
3	L	106	 83% 17%
4	G	120	 92% 8%
4	I	120	 92% 8%
4	J	120	 92% 8%
5	M	2	 50% 50%
5	O	2	 50% 50%
5	Q	2	 50% 50%
6	N	5	 20% 60% 40%
6	P	5	 20% 60% 40%
6	R	5	 20% 60% 40%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 13584 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 Bundibugyo virus GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	1781	1147	299	329	6	0	0
1	B	224	1781	1147	299	329	6	0	0
1	C	224	1781	1147	299	329	6	0	0

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	ILE	-	expression tag	UNP B8XCNO
A	314	ASP	-	expression tag	UNP B8XCNO
A	315	ILE	-	expression tag	UNP B8XCNO
A	316	SER	-	expression tag	UNP B8XCNO
A	317	GLU	-	expression tag	UNP B8XCNO
A	318	SER	-	expression tag	UNP B8XCNO
A	319	THR	-	expression tag	UNP B8XCNO
A	320	GLU	-	expression tag	UNP B8XCNO
A	321	PRO	-	expression tag	UNP B8XCNO
A	322	GLY	-	expression tag	UNP B8XCNO
A	323	PRO	-	expression tag	UNP B8XCNO
A	324	LEU	-	expression tag	UNP B8XCNO
A	325	THR	-	expression tag	UNP B8XCNO
A	326	ASN	-	expression tag	UNP B8XCNO
A	327	THR	-	expression tag	UNP B8XCNO
A	328	THR	-	expression tag	UNP B8XCNO
A	329	ARG	-	expression tag	UNP B8XCNO
A	330	GLY	-	expression tag	UNP B8XCNO
A	331	ALA	-	expression tag	UNP B8XCNO
A	332	ALA	-	expression tag	UNP B8XCNO
A	333	ASN	-	expression tag	UNP B8XCNO
A	334	LEU	-	expression tag	UNP B8XCNO
A	335	LEU	-	expression tag	UNP B8XCNO
A	336	THR	-	expression tag	UNP B8XCNO

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Chain	Residue	Modelled	Actual	Comment	Reference
A	337	GLY	-	expression tag	UNP B8XCNO
A	338	SER	-	expression tag	UNP B8XCNO
A	339	ARG	-	expression tag	UNP B8XCNO
A	340	ARG	-	expression tag	UNP B8XCNO
A	341	THR	-	expression tag	UNP B8XCNO
A	342	ARG	-	expression tag	UNP B8XCNO
A	343	ARG	-	expression tag	UNP B8XCNO
B	313	ILE	-	expression tag	UNP B8XCNO
B	314	ASP	-	expression tag	UNP B8XCNO
B	315	ILE	-	expression tag	UNP B8XCNO
B	316	SER	-	expression tag	UNP B8XCNO
B	317	GLU	-	expression tag	UNP B8XCNO
B	318	SER	-	expression tag	UNP B8XCNO
B	319	THR	-	expression tag	UNP B8XCNO
B	320	GLU	-	expression tag	UNP B8XCNO
B	321	PRO	-	expression tag	UNP B8XCNO
B	322	GLY	-	expression tag	UNP B8XCNO
B	323	PRO	-	expression tag	UNP B8XCNO
B	324	LEU	-	expression tag	UNP B8XCNO
B	325	THR	-	expression tag	UNP B8XCNO
B	326	ASN	-	expression tag	UNP B8XCNO
B	327	THR	-	expression tag	UNP B8XCNO
B	328	THR	-	expression tag	UNP B8XCNO
B	329	ARG	-	expression tag	UNP B8XCNO
B	330	GLY	-	expression tag	UNP B8XCNO
B	331	ALA	-	expression tag	UNP B8XCNO
B	332	ALA	-	expression tag	UNP B8XCNO
B	333	ASN	-	expression tag	UNP B8XCNO
B	334	LEU	-	expression tag	UNP B8XCNO
B	335	LEU	-	expression tag	UNP B8XCNO
B	336	THR	-	expression tag	UNP B8XCNO
B	337	GLY	-	expression tag	UNP B8XCNO
B	338	SER	-	expression tag	UNP B8XCNO
B	339	ARG	-	expression tag	UNP B8XCNO
B	340	ARG	-	expression tag	UNP B8XCNO
B	341	THR	-	expression tag	UNP B8XCNO
B	342	ARG	-	expression tag	UNP B8XCNO
B	343	ARG	-	expression tag	UNP B8XCNO
C	313	ILE	-	expression tag	UNP B8XCNO
C	314	ASP	-	expression tag	UNP B8XCNO
C	315	ILE	-	expression tag	UNP B8XCNO
C	316	SER	-	expression tag	UNP B8XCNO

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Chain	Residue	Modelled	Actual	Comment	Reference
C	317	GLU	-	expression tag	UNP B8XCN0
C	318	SER	-	expression tag	UNP B8XCN0
C	319	THR	-	expression tag	UNP B8XCN0
C	320	GLU	-	expression tag	UNP B8XCN0
C	321	PRO	-	expression tag	UNP B8XCN0
C	322	GLY	-	expression tag	UNP B8XCN0
C	323	PRO	-	expression tag	UNP B8XCN0
C	324	LEU	-	expression tag	UNP B8XCN0
C	325	THR	-	expression tag	UNP B8XCN0
C	326	ASN	-	expression tag	UNP B8XCN0
C	327	THR	-	expression tag	UNP B8XCN0
C	328	THR	-	expression tag	UNP B8XCN0
C	329	ARG	-	expression tag	UNP B8XCN0
C	330	GLY	-	expression tag	UNP B8XCN0
C	331	ALA	-	expression tag	UNP B8XCN0
C	332	ALA	-	expression tag	UNP B8XCN0
C	333	ASN	-	expression tag	UNP B8XCN0
C	334	LEU	-	expression tag	UNP B8XCN0
C	335	LEU	-	expression tag	UNP B8XCN0
C	336	THR	-	expression tag	UNP B8XCN0
C	337	GLY	-	expression tag	UNP B8XCN0
C	338	SER	-	expression tag	UNP B8XCN0
C	339	ARG	-	expression tag	UNP B8XCN0
C	340	ARG	-	expression tag	UNP B8XCN0
C	341	THR	-	expression tag	UNP B8XCN0
C	342	ARG	-	expression tag	UNP B8XCN0
C	343	ARG	-	expression tag	UNP B8XCN0

- Molecule 2 is a protein called Bundibugyo virus GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	115	Total	C	N	O	S	0	0
			912	579	159	168	6		
2	E	115	Total	C	N	O	S	0	0
			912	579	159	168	6		
2	F	115	Total	C	N	O	S	0	0
			912	579	159	168	6		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	641	VAL	-	insertion	UNP B8XCN0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	642	GLU	-	insertion	UNP B8XCNO
D	643	VAL	-	insertion	UNP B8XCNO
D	644	ASP	ASN	conflict	UNP B8XCNO
D	646	ASP	ASN	conflict	UNP B8XCNO
D	647	ASP	TRP	conflict	UNP B8XCNO
D	648	LYS	TRP	conflict	UNP B8XCNO
D	649	ALA	THR	conflict	UNP B8XCNO
D	652	SER	-	expression tag	UNP B8XCNO
D	653	HIS	-	expression tag	UNP B8XCNO
D	654	PRO	-	expression tag	UNP B8XCNO
D	655	GLN	-	expression tag	UNP B8XCNO
D	656	PHE	-	expression tag	UNP B8XCNO
D	657	GLU	-	expression tag	UNP B8XCNO
D	658	LYS	-	expression tag	UNP B8XCNO
D	659	GLY	-	expression tag	UNP B8XCNO
D	660	GLY	-	expression tag	UNP B8XCNO
D	661	GLY	-	expression tag	UNP B8XCNO
D	662	SER	-	expression tag	UNP B8XCNO
D	663	GLY	-	expression tag	UNP B8XCNO
D	664	GLY	-	expression tag	UNP B8XCNO
D	665	GLY	-	expression tag	UNP B8XCNO
D	666	SER	-	expression tag	UNP B8XCNO
D	667	GLY	-	expression tag	UNP B8XCNO
D	668	GLY	-	expression tag	UNP B8XCNO
D	669	GLY	-	expression tag	UNP B8XCNO
D	670	SER	-	expression tag	UNP B8XCNO
D	671	TRP	-	expression tag	UNP B8XCNO
D	672	SER	-	expression tag	UNP B8XCNO
D	673	HIS	-	expression tag	UNP B8XCNO
D	674	PRO	-	expression tag	UNP B8XCNO
D	675	GLN	-	expression tag	UNP B8XCNO
D	676	PHE	-	expression tag	UNP B8XCNO
D	677	GLU	-	expression tag	UNP B8XCNO
D	678	LYS	-	expression tag	UNP B8XCNO
E	641	VAL	-	insertion	UNP B8XCNO
E	642	GLU	-	insertion	UNP B8XCNO
E	643	VAL	-	insertion	UNP B8XCNO
E	644	ASP	ASN	conflict	UNP B8XCNO
E	646	ASP	ASN	conflict	UNP B8XCNO
E	647	ASP	TRP	conflict	UNP B8XCNO
E	648	LYS	TRP	conflict	UNP B8XCNO
E	649	ALA	THR	conflict	UNP B8XCNO

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Chain	Residue	Modelled	Actual	Comment	Reference
E	652	SER	-	expression tag	UNP B8XCNO
E	653	HIS	-	expression tag	UNP B8XCNO
E	654	PRO	-	expression tag	UNP B8XCNO
E	655	GLN	-	expression tag	UNP B8XCNO
E	656	PHE	-	expression tag	UNP B8XCNO
E	657	GLU	-	expression tag	UNP B8XCNO
E	658	LYS	-	expression tag	UNP B8XCNO
E	659	GLY	-	expression tag	UNP B8XCNO
E	660	GLY	-	expression tag	UNP B8XCNO
E	661	GLY	-	expression tag	UNP B8XCNO
E	662	SER	-	expression tag	UNP B8XCNO
E	663	GLY	-	expression tag	UNP B8XCNO
E	664	GLY	-	expression tag	UNP B8XCNO
E	665	GLY	-	expression tag	UNP B8XCNO
E	666	SER	-	expression tag	UNP B8XCNO
E	667	GLY	-	expression tag	UNP B8XCNO
E	668	GLY	-	expression tag	UNP B8XCNO
E	669	GLY	-	expression tag	UNP B8XCNO
E	670	SER	-	expression tag	UNP B8XCNO
E	671	TRP	-	expression tag	UNP B8XCNO
E	672	SER	-	expression tag	UNP B8XCNO
E	673	HIS	-	expression tag	UNP B8XCNO
E	674	PRO	-	expression tag	UNP B8XCNO
E	675	GLN	-	expression tag	UNP B8XCNO
E	676	PHE	-	expression tag	UNP B8XCNO
E	677	GLU	-	expression tag	UNP B8XCNO
E	678	LYS	-	expression tag	UNP B8XCNO
F	641	VAL	-	insertion	UNP B8XCNO
F	642	GLU	-	insertion	UNP B8XCNO
F	643	VAL	-	insertion	UNP B8XCNO
F	644	ASP	ASN	conflict	UNP B8XCNO
F	646	ASP	ASN	conflict	UNP B8XCNO
F	647	ASP	TRP	conflict	UNP B8XCNO
F	648	LYS	TRP	conflict	UNP B8XCNO
F	649	ALA	THR	conflict	UNP B8XCNO
F	652	SER	-	expression tag	UNP B8XCNO
F	653	HIS	-	expression tag	UNP B8XCNO
F	654	PRO	-	expression tag	UNP B8XCNO
F	655	GLN	-	expression tag	UNP B8XCNO
F	656	PHE	-	expression tag	UNP B8XCNO
F	657	GLU	-	expression tag	UNP B8XCNO
F	658	LYS	-	expression tag	UNP B8XCNO

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Chain	Residue	Modelled	Actual	Comment	Reference
F	659	GLY	-	expression tag	UNP B8XCNO
F	660	GLY	-	expression tag	UNP B8XCNO
F	661	GLY	-	expression tag	UNP B8XCNO
F	662	SER	-	expression tag	UNP B8XCNO
F	663	GLY	-	expression tag	UNP B8XCNO
F	664	GLY	-	expression tag	UNP B8XCNO
F	665	GLY	-	expression tag	UNP B8XCNO
F	666	SER	-	expression tag	UNP B8XCNO
F	667	GLY	-	expression tag	UNP B8XCNO
F	668	GLY	-	expression tag	UNP B8XCNO
F	669	GLY	-	expression tag	UNP B8XCNO
F	670	SER	-	expression tag	UNP B8XCNO
F	671	TRP	-	expression tag	UNP B8XCNO
F	672	SER	-	expression tag	UNP B8XCNO
F	673	HIS	-	expression tag	UNP B8XCNO
F	674	PRO	-	expression tag	UNP B8XCNO
F	675	GLN	-	expression tag	UNP B8XCNO
F	676	PHE	-	expression tag	UNP B8XCNO
F	677	GLU	-	expression tag	UNP B8XCNO
F	678	LYS	-	expression tag	UNP B8XCNO

- Molecule 3 is a protein called Antibody ADI-15878 Fab, light chain.

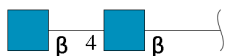
Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
3	H	106	Total	C	N	O	S	0	0
			798	501	128	167	2		
3	K	106	Total	C	N	O	S	0	0
			798	501	128	167	2		
3	L	106	Total	C	N	O	S	0	0
			798	501	128	167	2		

- Molecule 4 is a protein called Antibody ADI-15878 Fab, heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
4	G	120	Total	C	N	O	S	0	0
			920	583	159	174	4		
4	I	120	Total	C	N	O	S	0	0
			920	583	159	174	4		
4	J	120	Total	C	N	O	S	0	0
			920	583	159	174	4		

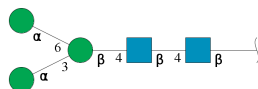
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

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



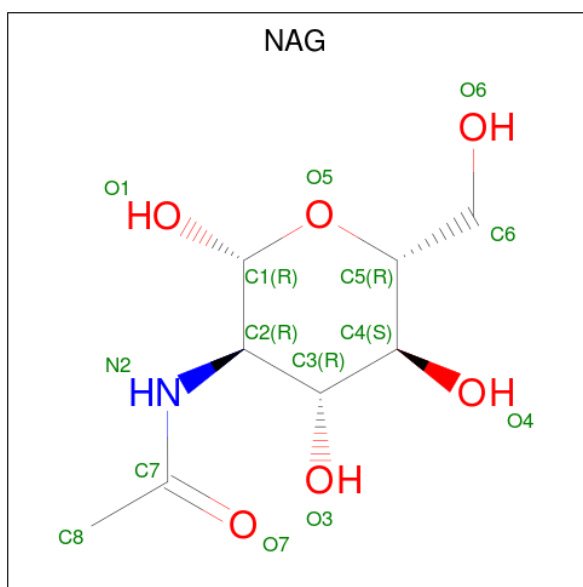
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	2	28	16	2	10	0	0
5	O	2	28	16	2	10	0	0
5	Q	2	28	16	2	10	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O		
6	N	5	61	34	2	25	0	0
6	P	5	61	34	2	25	0	0
6	R	5	61	34	2	25	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

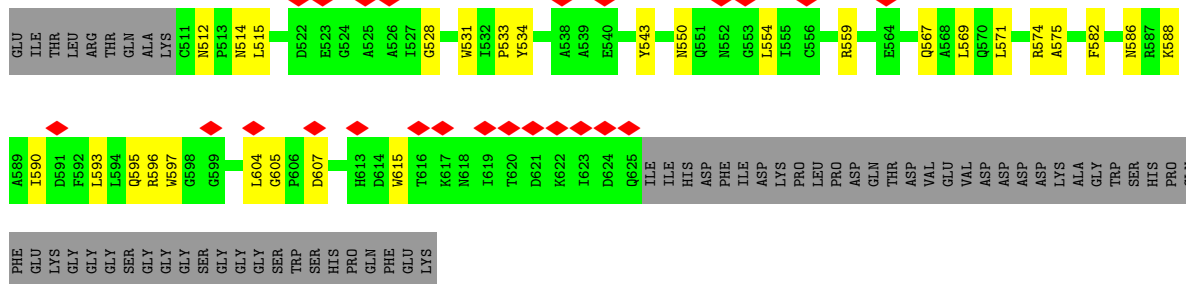


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 14	8	1	5	0
7	D	1	Total 14	8	1	5	0
7	B	1	Total 14	8	1	5	0
7	E	1	Total 14	8	1	5	0
7	C	1	Total 14	8	1	5	0
7	F	1	Total 14	8	1	5	0

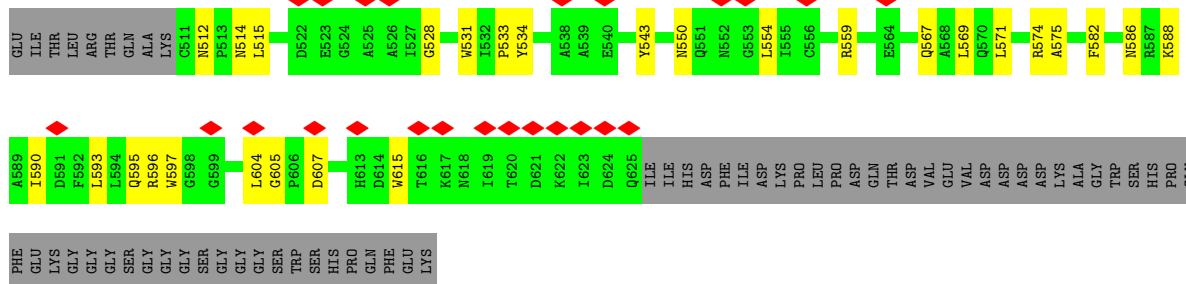


LYS ASN THR THR THR THR LEU SER SER GLU GLU LEU LEU SER VAL ILE PHE VAL PRO ILE ASP ILE SER GLU SER THR THR GLU PRO GLY PRO PRO LEU THR ASN THR THR ARG ARG ARG ARG ARG

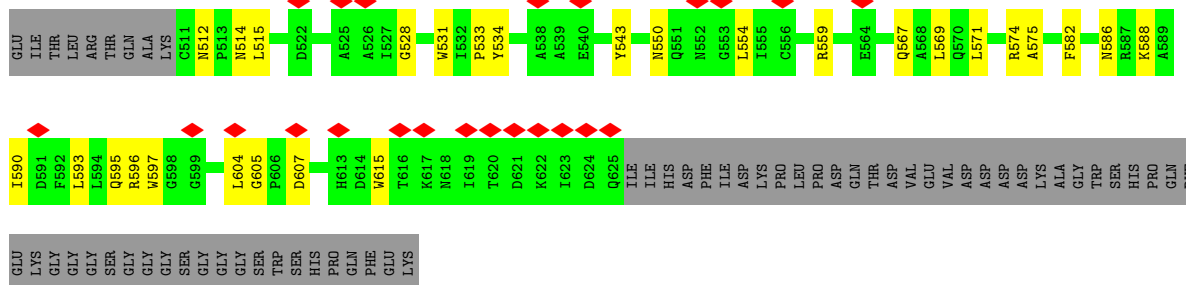
• Molecule 2: Bundibugyo virus GP2



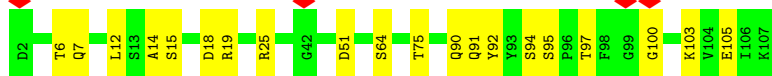
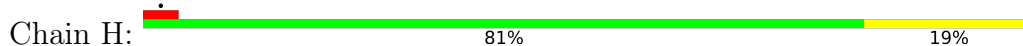
• Molecule 2: Bundibugyo virus GP2




• Molecule 2: Bundibugyo virus GP2

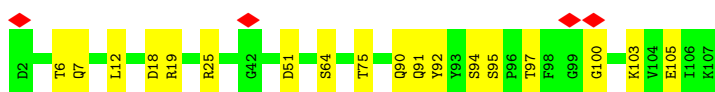


• Molecule 3: Antibody ADI-15878 Fab, light chain




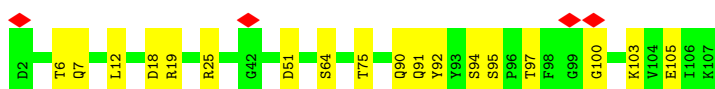
- Molecule 3: Antibody ADI-15878 Fab, light chain

Chain K:  83% 17%

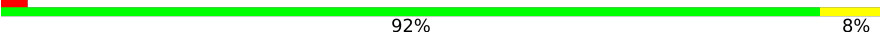


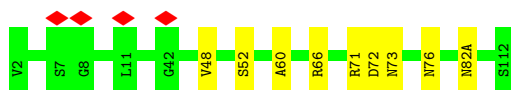
- Molecule 3: Antibody ADI-15878 Fab, light chain

Chain L:  83% 17%



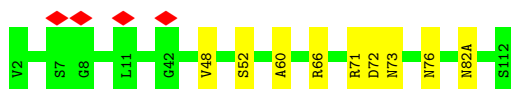
- Molecule 4: Antibody ADI-15878 Fab, heavy chain

Chain G:  92% 8%




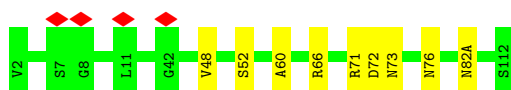
- Molecule 4: Antibody ADI-15878 Fab, heavy chain

Chain I:  92% 8%



- Molecule 4: Antibody ADI-15878 Fab, heavy chain

Chain J:  92% 8%



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

Chain M:  50% 50%



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

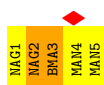
Chain O:  50% 50%



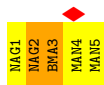
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



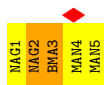
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	35961	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	38167	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0393	Depositor
Map size (Å)	429.68, 429.68, 429.68	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/1827	0.60	0/2485
1	B	0.41	0/1827	0.60	0/2485
1	C	0.41	0/1827	0.60	0/2485
2	D	0.44	0/935	0.62	0/1274
2	E	0.45	0/935	0.62	0/1274
2	F	0.45	0/935	0.62	0/1274
3	H	0.40	0/816	0.62	0/1109
3	K	0.40	0/816	0.62	0/1109
3	L	0.40	0/816	0.62	0/1109
4	G	0.41	0/943	0.61	0/1279
4	I	0.41	0/943	0.61	0/1279
4	J	0.41	0/943	0.60	0/1279
All	All	0.42	0/13563	0.61	0/18441

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 [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	1781	0	1730	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1781	0	1730	28	0
1	C	1781	0	1730	28	0
2	D	912	0	875	63	0
2	E	912	0	875	63	0
2	F	912	0	875	64	0
3	H	798	0	767	12	0
3	K	798	0	767	11	0
3	L	798	0	767	10	0
4	G	920	0	881	5	0
4	I	920	0	881	5	0
4	J	920	0	881	5	0
5	M	28	0	25	1	0
5	O	28	0	25	1	0
5	Q	28	0	25	1	0
6	N	61	0	52	2	0
6	P	61	0	52	2	0
6	R	61	0	52	2	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	4	0
7	E	14	0	13	4	0
7	F	14	0	13	4	0
All	All	13584	0	13068	229	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 9.

The worst 5 of 229 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:533:PRO:HA	2:F:574:ARG:HH22	1.39	0.88
2:E:574:ARG:HH22	2:F:533:PRO:HA	1.38	0.88
2:D:574:ARG:HH22	2:E:533:PRO:HA	1.38	0.87
1:C:98:ASN:ND2	2:F:582:PHE:HD1	1.73	0.86
1:B:98:ASN:ND2	2:E:582:PHE:HD1	1.73	0.86

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	216/311 (70%)	192 (89%)	24 (11%)	0	100	100
1	B	216/311 (70%)	192 (89%)	24 (11%)	0	100	100
1	C	216/311 (70%)	192 (89%)	24 (11%)	0	100	100
2	D	113/177 (64%)	91 (80%)	22 (20%)	0	100	100
2	E	113/177 (64%)	91 (80%)	22 (20%)	0	100	100
2	F	113/177 (64%)	91 (80%)	22 (20%)	0	100	100
3	H	104/106 (98%)	89 (86%)	15 (14%)	0	100	100
3	K	104/106 (98%)	89 (86%)	15 (14%)	0	100	100
3	L	104/106 (98%)	89 (86%)	15 (14%)	0	100	100
4	G	118/120 (98%)	104 (88%)	14 (12%)	0	100	100
4	I	118/120 (98%)	104 (88%)	14 (12%)	0	100	100
4	J	118/120 (98%)	104 (88%)	14 (12%)	0	100	100
All	All	1653/2142 (77%)	1428 (86%)	225 (14%)	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	194/272 (71%)	194 (100%)	0	100	100
1	B	194/272 (71%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	194/272 (71%)	194 (100%)	0	100	100
2	D	96/146 (66%)	96 (100%)	0	100	100
2	E	96/146 (66%)	96 (100%)	0	100	100
2	F	96/146 (66%)	96 (100%)	0	100	100
3	H	91/91 (100%)	91 (100%)	0	100	100
3	K	91/91 (100%)	91 (100%)	0	100	100
3	L	91/91 (100%)	91 (100%)	0	100	100
4	G	95/95 (100%)	95 (100%)	0	100	100
4	I	95/95 (100%)	95 (100%)	0	100	100
4	J	95/95 (100%)	95 (100%)	0	100	100
All	All	1428/1812 (79%)	1428 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	62	GLN
1	C	62	GLN
3	L	90	GLN

### 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](#)

21 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	M	1	5,1	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
5	NAG	M	2	5	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	N	1	6,2	14,14,15	0.60	0	17,19,21	0.75	0
6	NAG	N	2	6	14,14,15	0.53	0	17,19,21	0.98	2 (11%)
6	BMA	N	3	6	11,11,12	0.41	0	15,15,17	1.21	1 (6%)
6	MAN	N	4	6	11,11,12	0.61	0	15,15,17	1.22	2 (13%)
6	MAN	N	5	6	11,11,12	0.53	0	15,15,17	0.95	2 (13%)
5	NAG	O	1	5,1	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
5	NAG	O	2	5	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	P	1	6,2	14,14,15	0.60	0	17,19,21	0.75	0
6	NAG	P	2	6	14,14,15	0.52	0	17,19,21	0.97	2 (11%)
6	BMA	P	3	6	11,11,12	0.41	0	15,15,17	1.21	1 (6%)
6	MAN	P	4	6	11,11,12	0.61	0	15,15,17	1.21	2 (13%)
6	MAN	P	5	6	11,11,12	0.53	0	15,15,17	0.95	2 (13%)
5	NAG	Q	1	5,1	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
5	NAG	Q	2	5	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	R	1	6,2	14,14,15	0.60	0	17,19,21	0.75	0
6	NAG	R	2	6	14,14,15	0.53	0	17,19,21	0.98	2 (11%)
6	BMA	R	3	6	11,11,12	0.40	0	15,15,17	1.21	1 (6%)
6	MAN	R	4	6	11,11,12	0.62	0	15,15,17	1.21	2 (13%)
6	MAN	R	5	6	11,11,12	0.53	0	15,15,17	0.95	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	5,1	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
6	NAG	N	1	6,2	-	3/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	N	4	6	-	2/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
6	NAG	P	1	6,2	-	3/6/23/26	0/1/1/1
6	NAG	P	2	6	-	3/6/23/26	0/1/1/1
6	BMA	P	3	6	-	2/2/19/22	0/1/1/1
6	MAN	P	4	6	-	2/2/19/22	0/1/1/1
6	MAN	P	5	6	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	1/6/23/26	0/1/1/1
6	NAG	R	1	6,2	-	3/6/23/26	0/1/1/1
6	NAG	R	2	6	-	3/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	2/2/19/22	0/1/1/1
6	MAN	R	5	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C2-N2-C7	4.19	128.87	122.90
5	O	1	NAG	C2-N2-C7	4.18	128.86	122.90
5	Q	1	NAG	C2-N2-C7	4.18	128.86	122.90
6	N	4	MAN	C1-O5-C5	3.25	116.60	112.19
6	P	4	MAN	C1-O5-C5	3.23	116.57	112.19

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

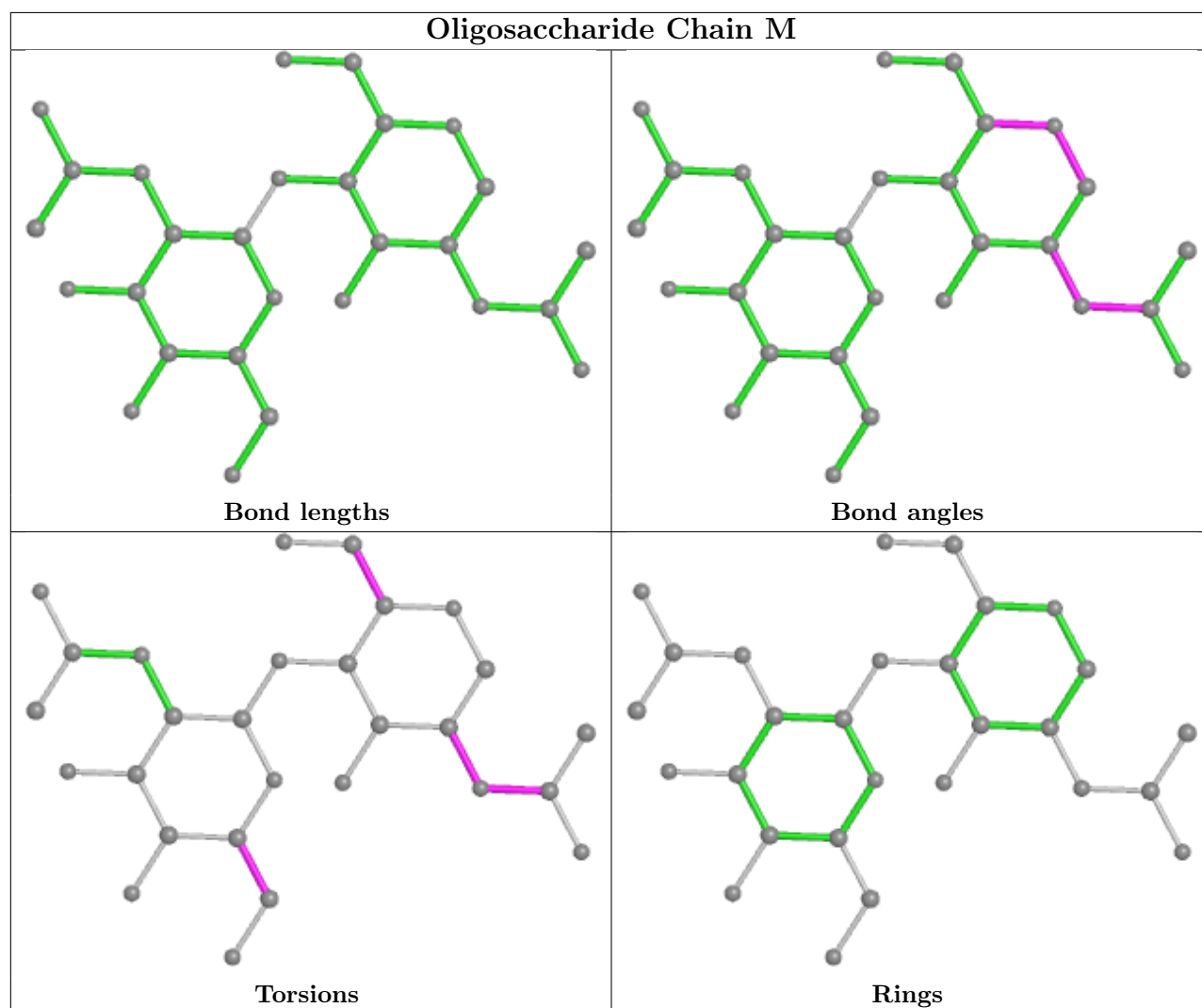
Mol	Chain	Res	Type	Atoms
6	N	3	BMA	C4-C5-C6-O6
6	P	3	BMA	C4-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6

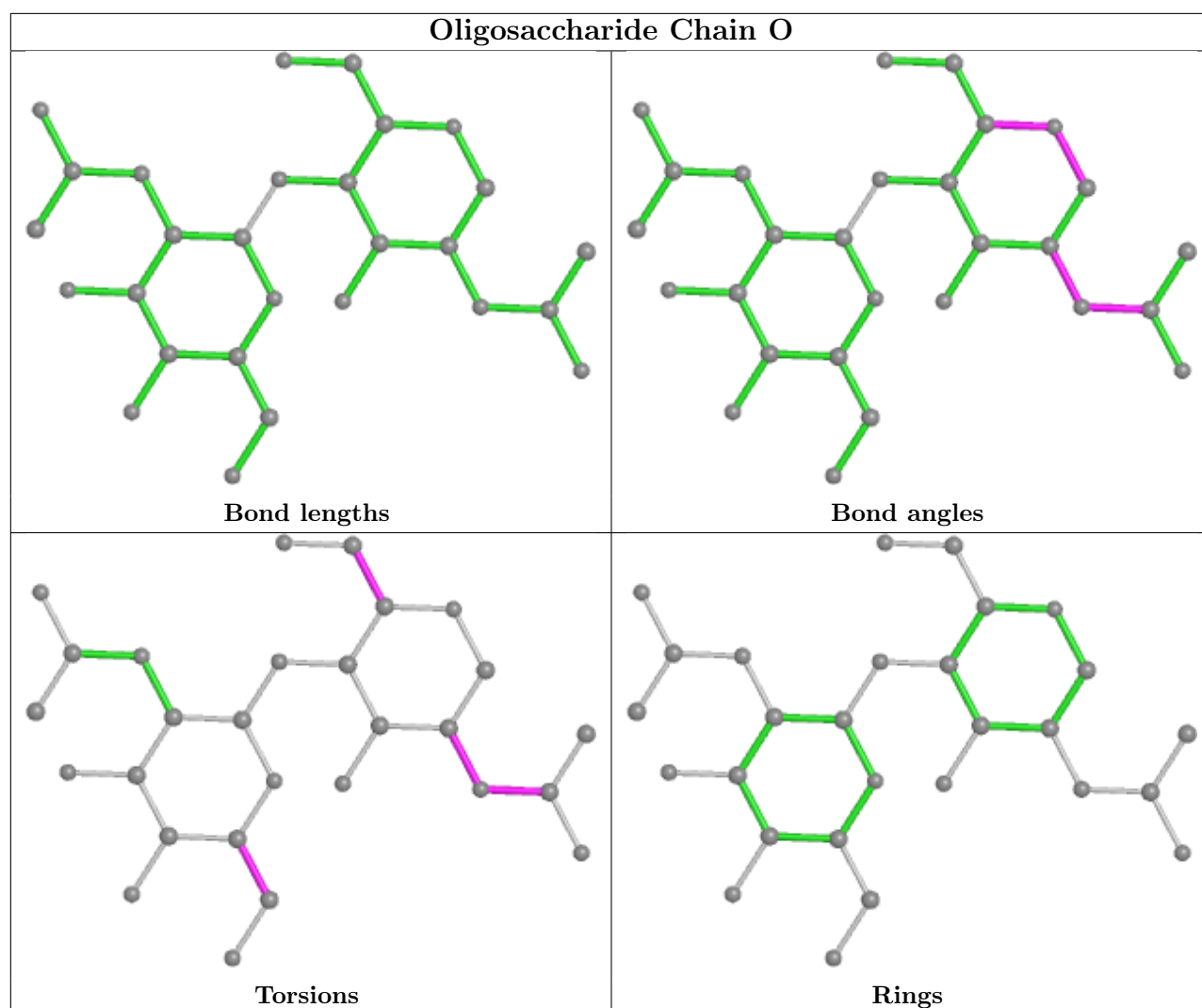
There are no ring outliers.

12 monomers are involved in 9 short contacts:

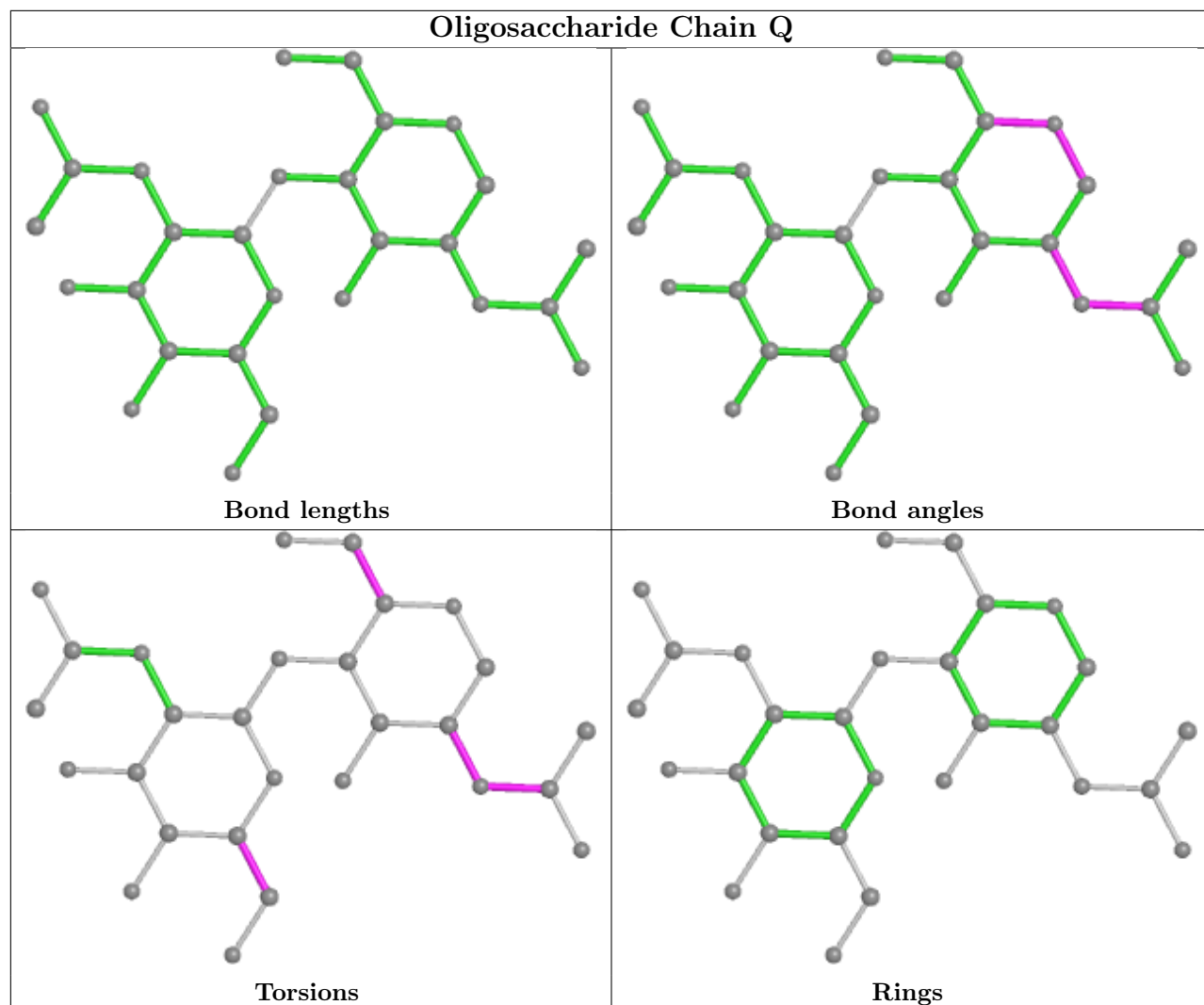
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	2	NAG	2	0
6	P	3	BMA	1	0
5	O	1	NAG	1	0
6	R	3	BMA	1	0
6	R	1	NAG	1	0
6	R	2	NAG	2	0
5	M	1	NAG	1	0
6	N	1	NAG	1	0
6	N	2	NAG	2	0
6	N	3	BMA	1	0
5	Q	1	NAG	1	0
6	P	1	NAG	1	0

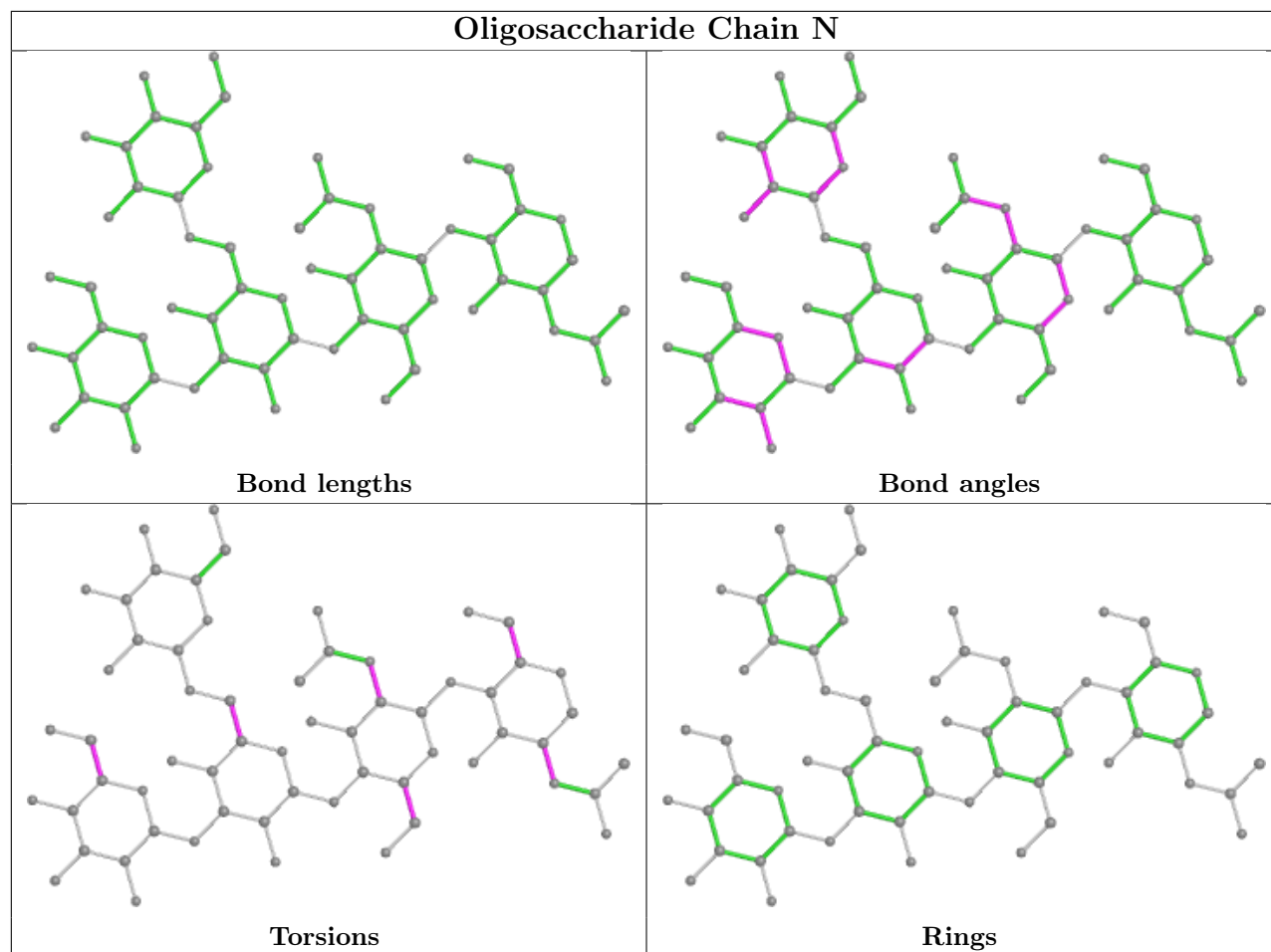
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

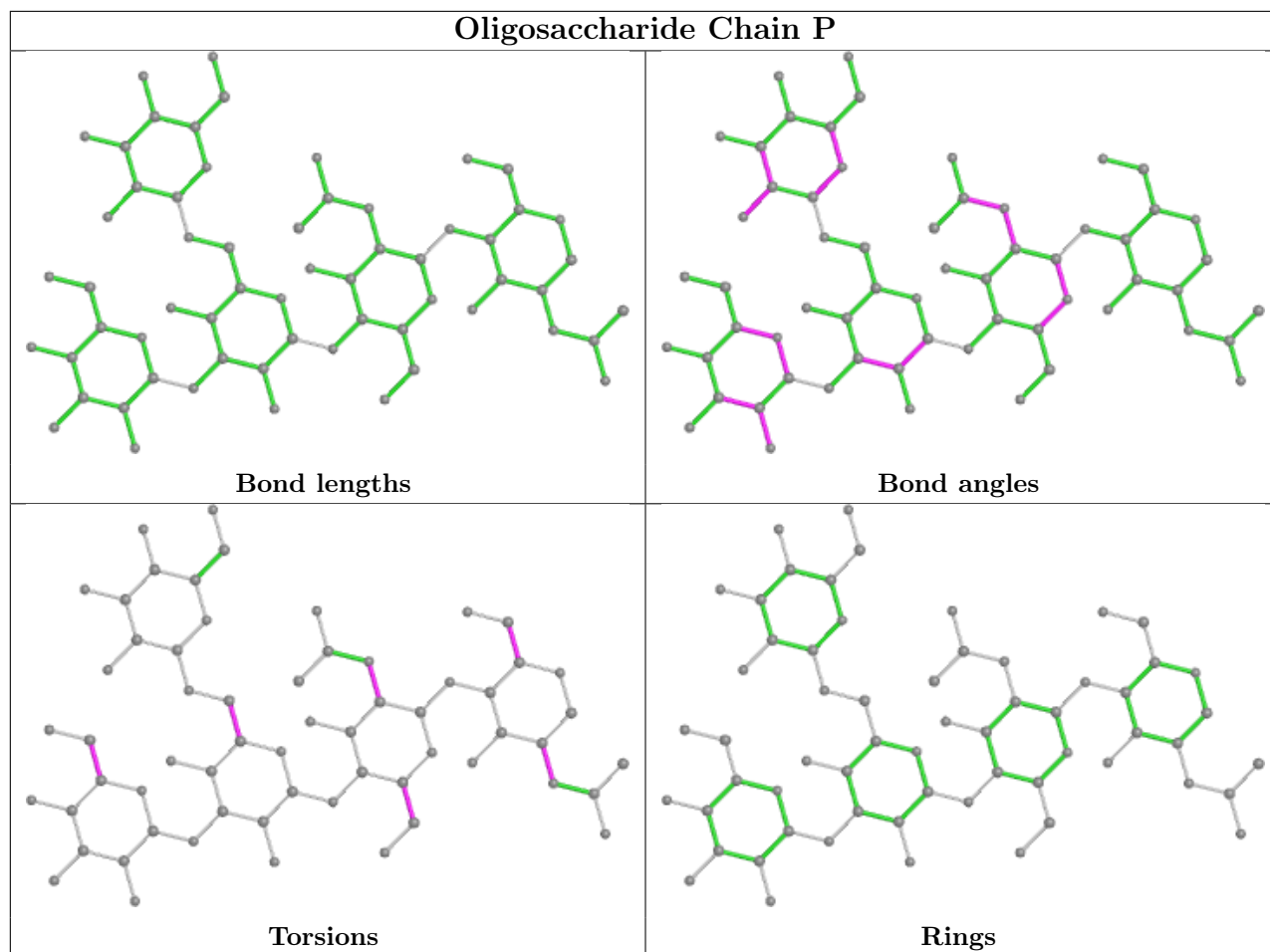


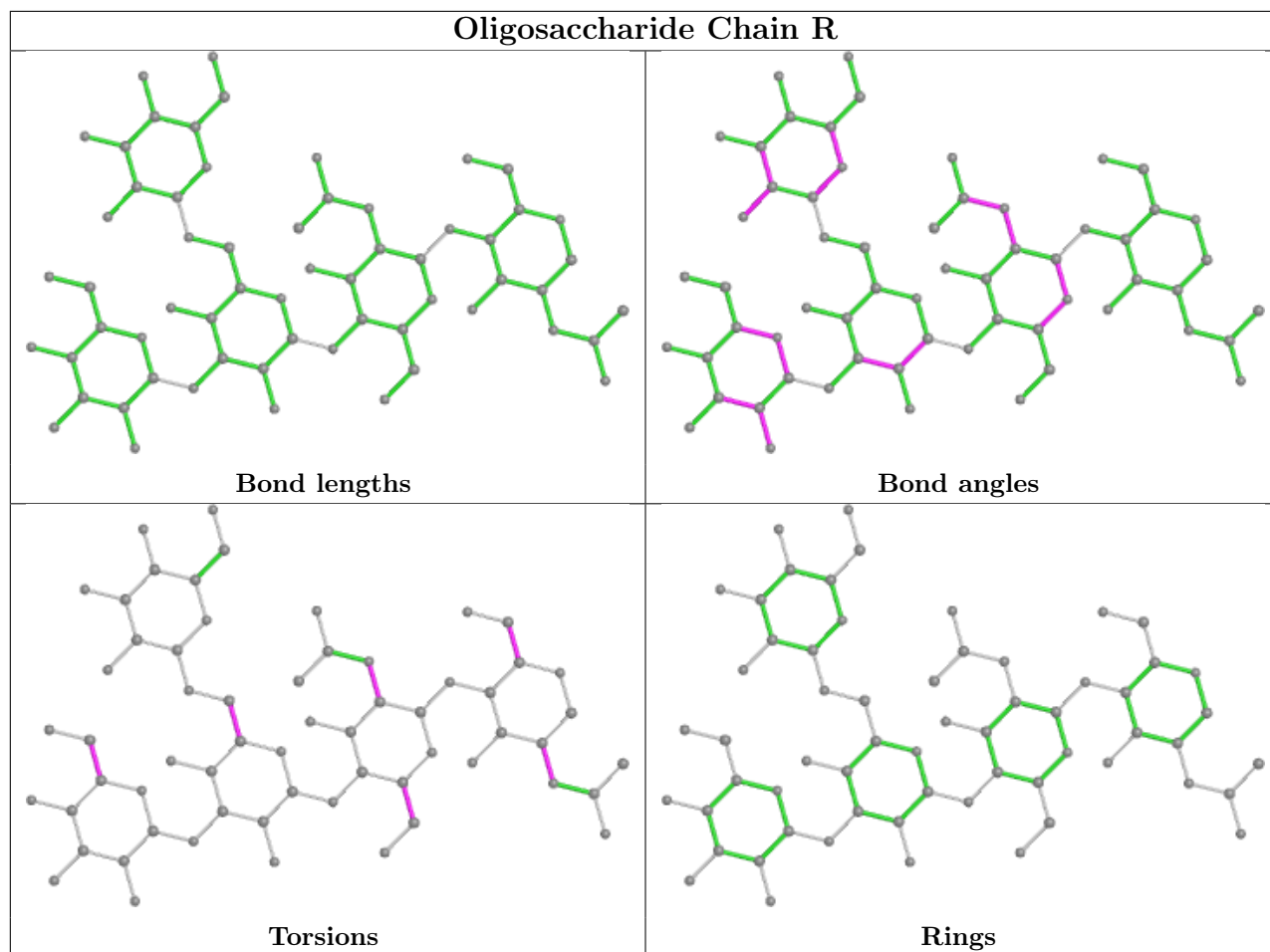












## 5.6 Ligand geometry [i](#)

6 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	E	701	2	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
7	NAG	D	701	2	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
7	NAG	A	403	1	14,14,15	0.35	0	17,19,21	0.44	0
7	NAG	F	701	2	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
7	NAG	C	403	1	14,14,15	0.36	0	17,19,21	0.44	0
7	NAG	B	403	1	14,14,15	0.35	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
7	NAG	E	701	2	-	2/6/23/26	0/1/1/1
7	NAG	D	701	2	-	2/6/23/26	0/1/1/1
7	NAG	A	403	1	-	1/6/23/26	0/1/1/1
7	NAG	F	701	2	-	2/6/23/26	0/1/1/1
7	NAG	C	403	1	-	1/6/23/26	0/1/1/1
7	NAG	B	403	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	701	NAG	C1-C2	2.88	1.56	1.52
7	D	701	NAG	C1-C2	2.85	1.56	1.52
7	F	701	NAG	C1-C2	2.83	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	NAG	C1-O5-C5	2.41	115.45	112.19
7	E	701	NAG	C1-O5-C5	2.40	115.45	112.19
7	F	701	NAG	C1-O5-C5	2.40	115.45	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	701	NAG	O5-C5-C6-O6
7	E	701	NAG	O5-C5-C6-O6
7	F	701	NAG	O5-C5-C6-O6
7	A	403	NAG	O5-C5-C6-O6
7	B	403	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	701	NAG	4	0
7	D	701	NAG	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	701	NAG	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

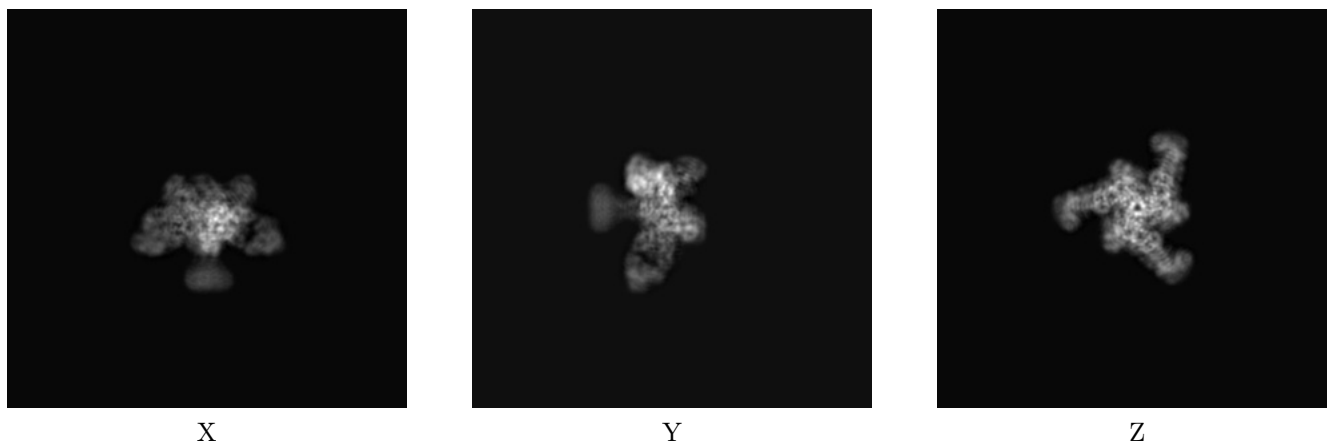
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8936. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

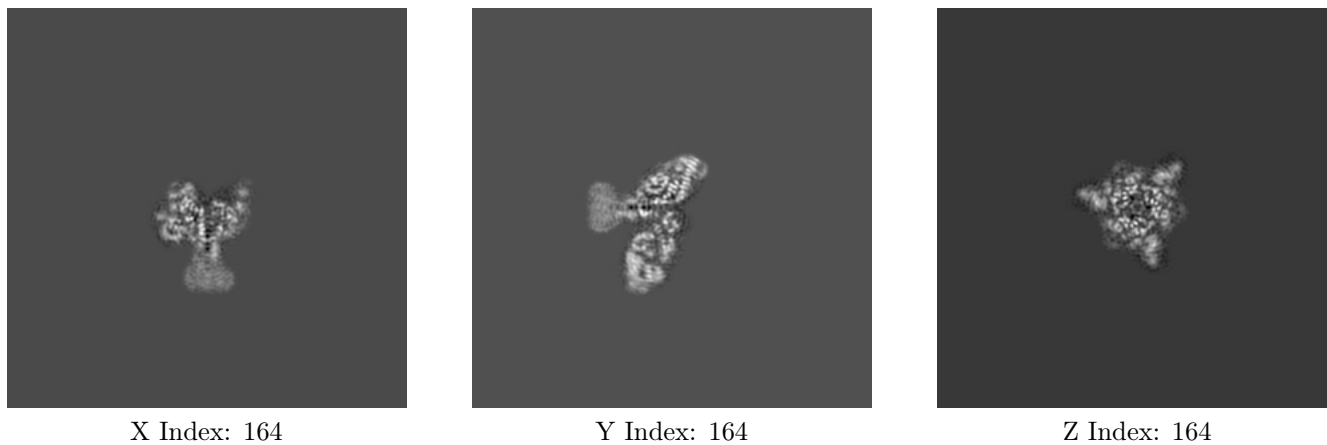
#### 6.1.1 Primary map



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

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

#### 6.2.1 Primary map



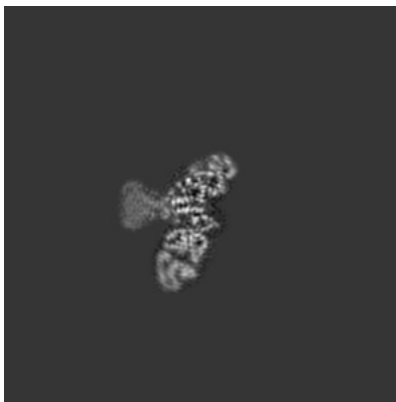
The images above show central slices of the map in three orthogonal directions.

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

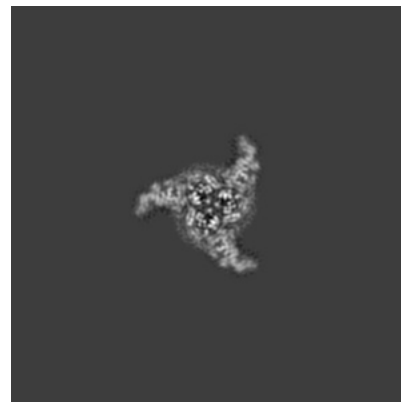
### 6.3.1 Primary map



X Index: 188



Y Index: 167



Z Index: 155

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

## 6.4 Orthogonal surface views [i](#)

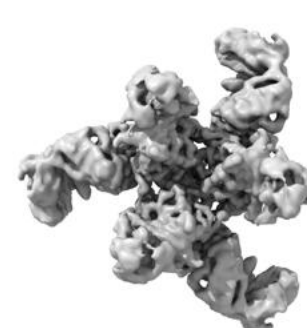
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0393. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



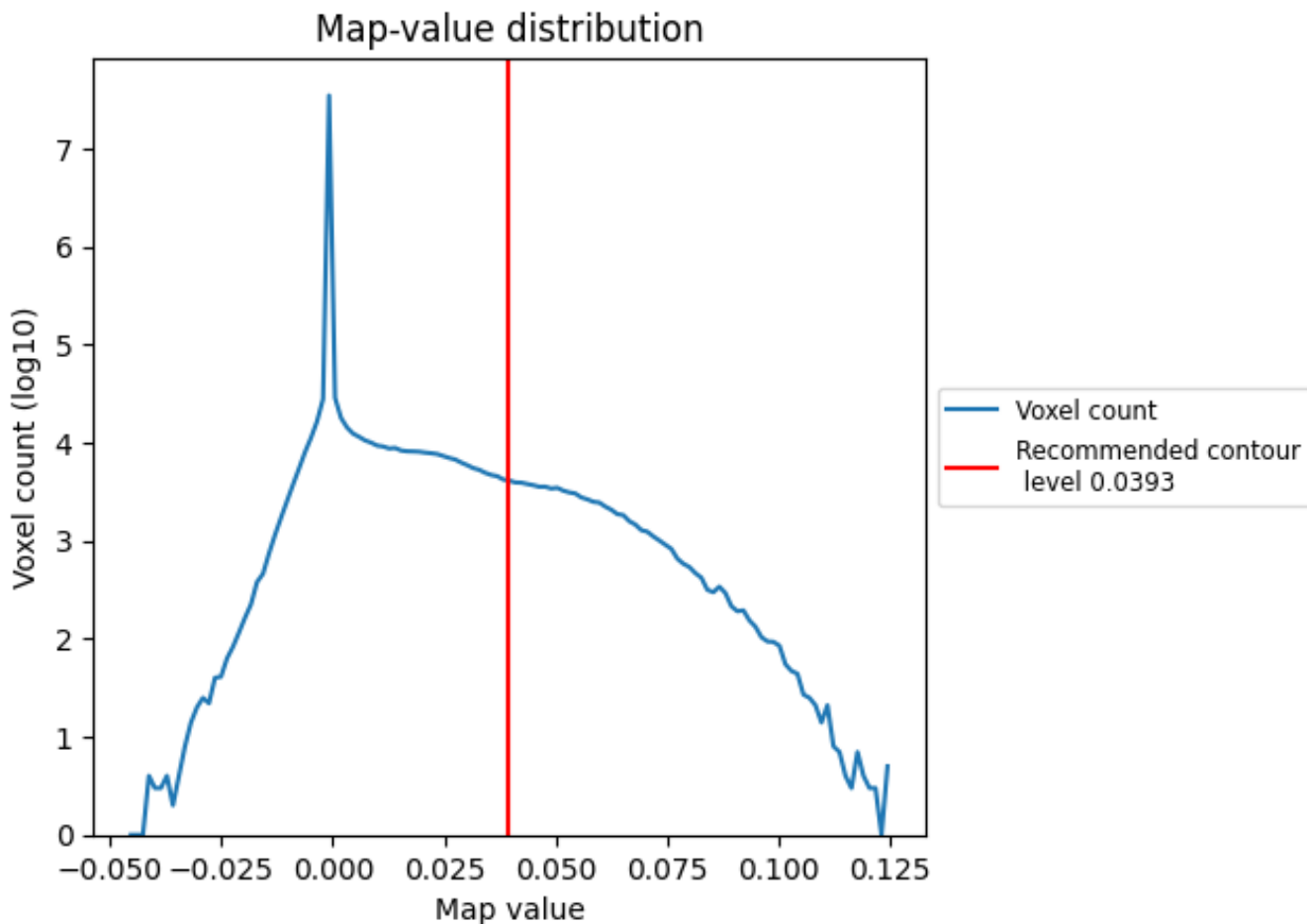
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

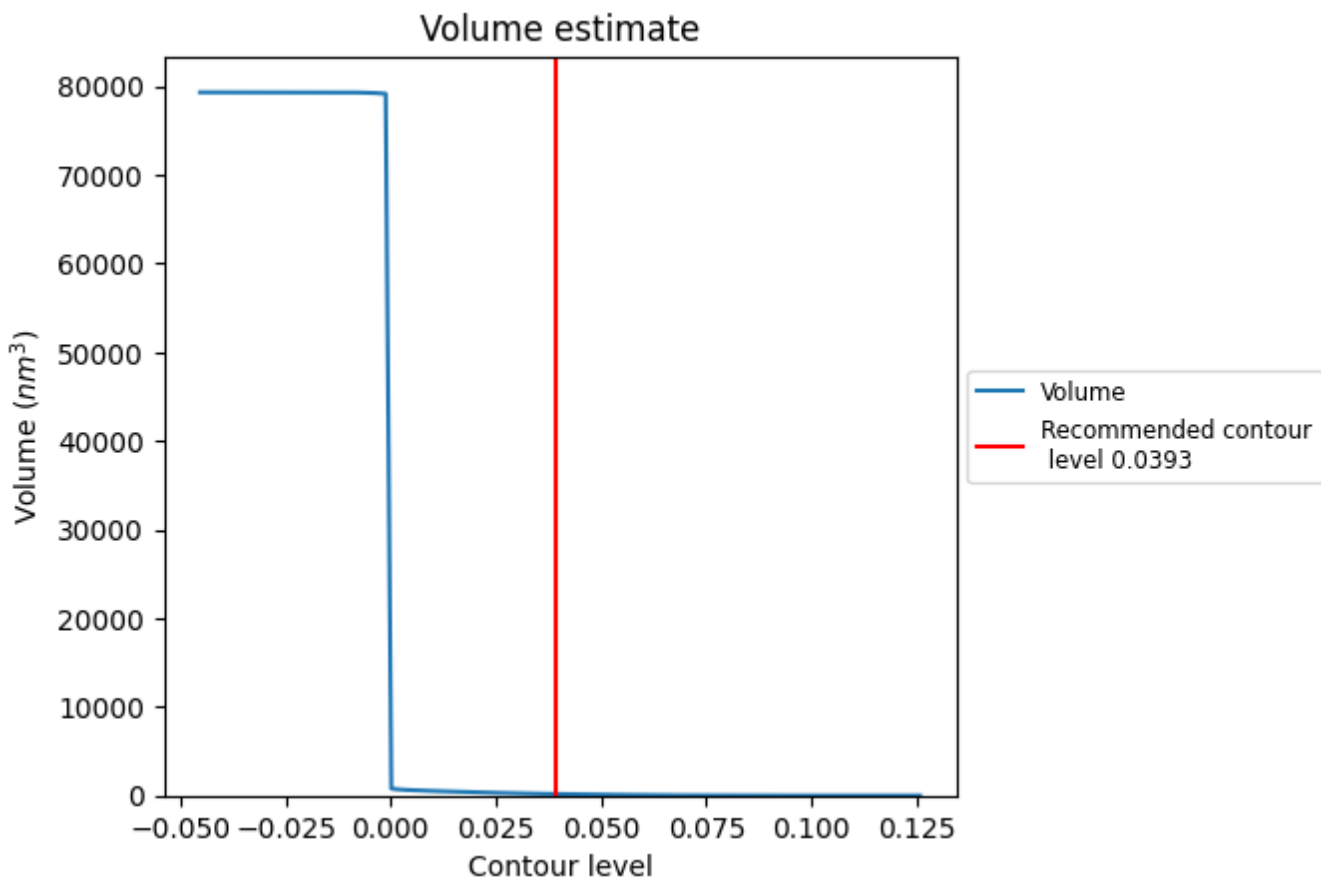
This section contains the results of statistical analysis of the map.

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



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

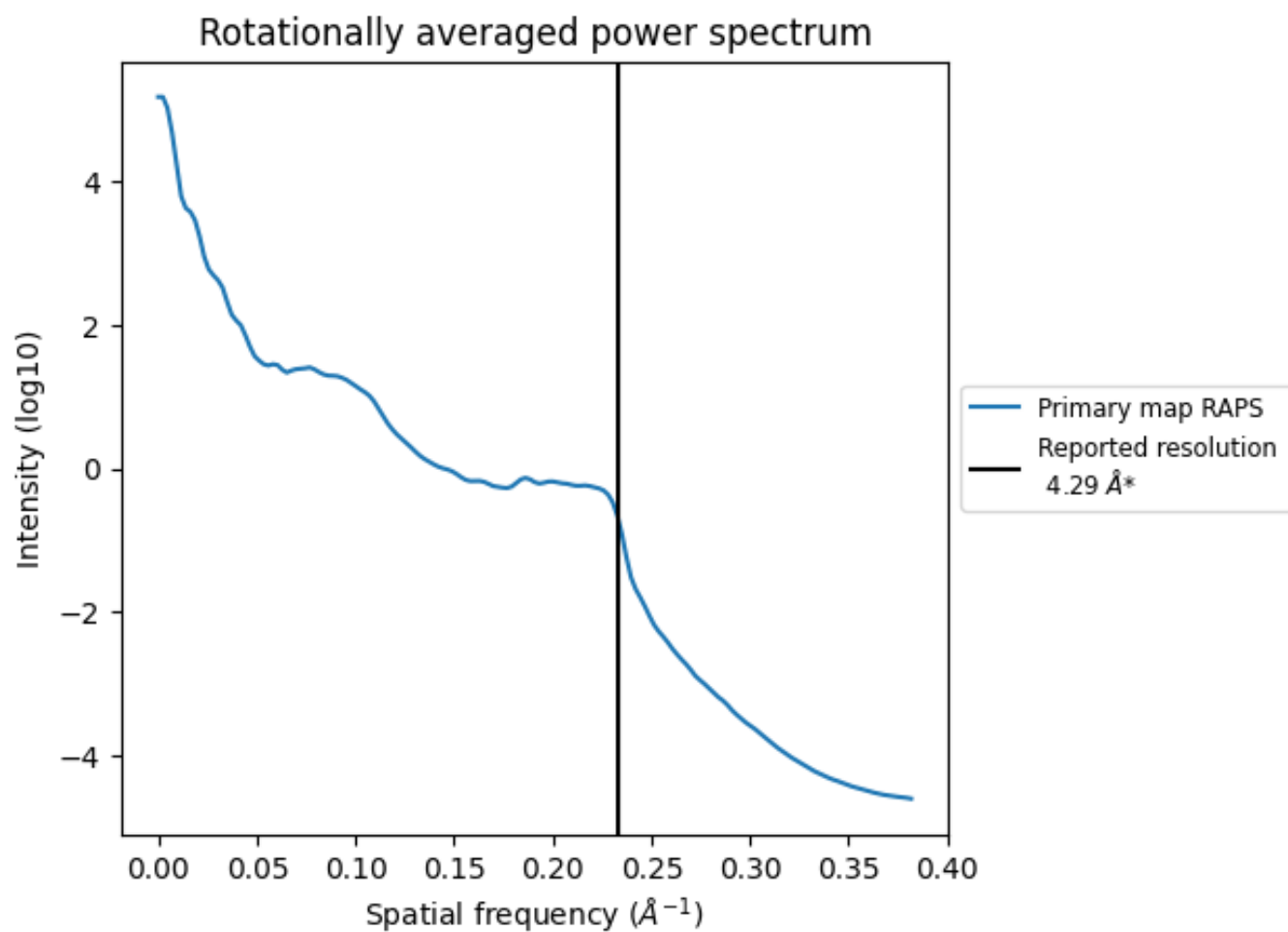
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 173  $\text{nm}^3$ ; this corresponds to an approximate mass of 156 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](#)

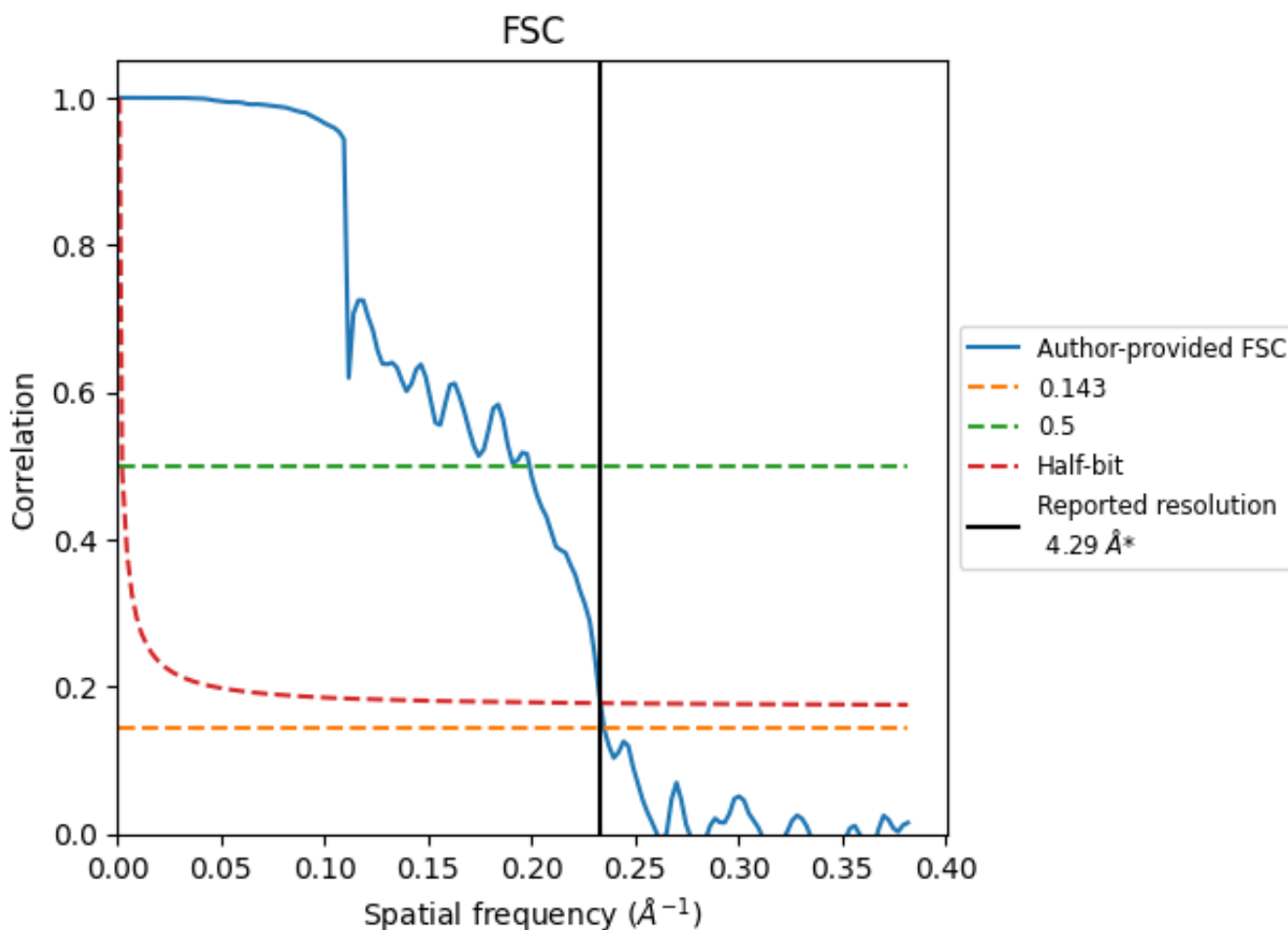


\*Reported resolution corresponds to spatial frequency of  $0.233 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

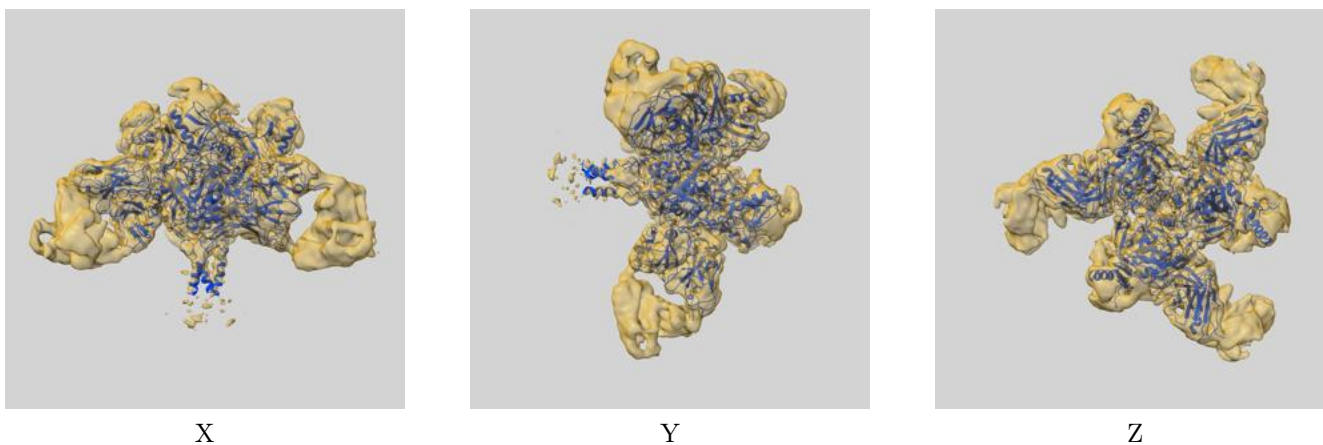
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.29	-	-
Author-provided FSC curve	4.26	5.03	4.29
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

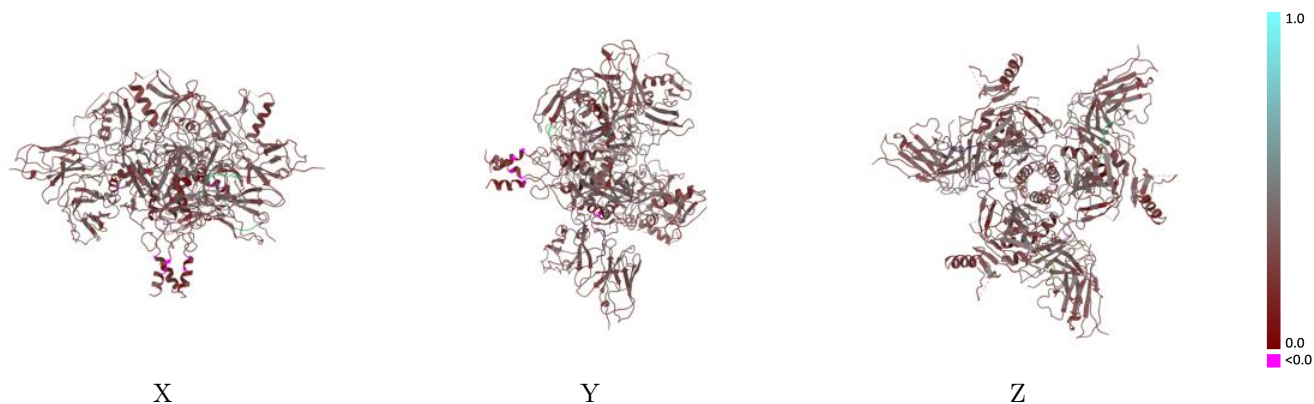
This section contains information regarding the fit between EMDB map EMD-8936 and PDB model 6DZM. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



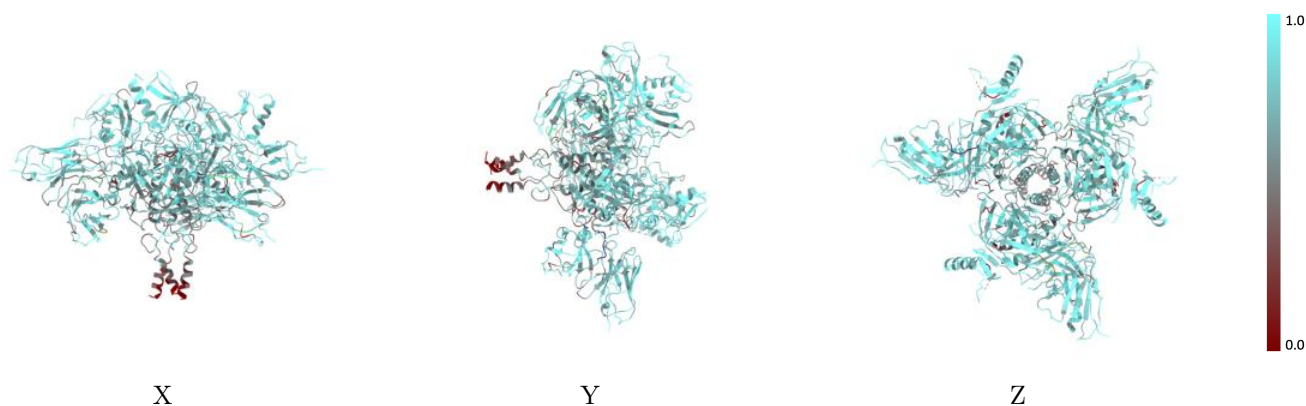
The images above show the 3D surface view of the map at the recommended contour level 0.0393 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



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

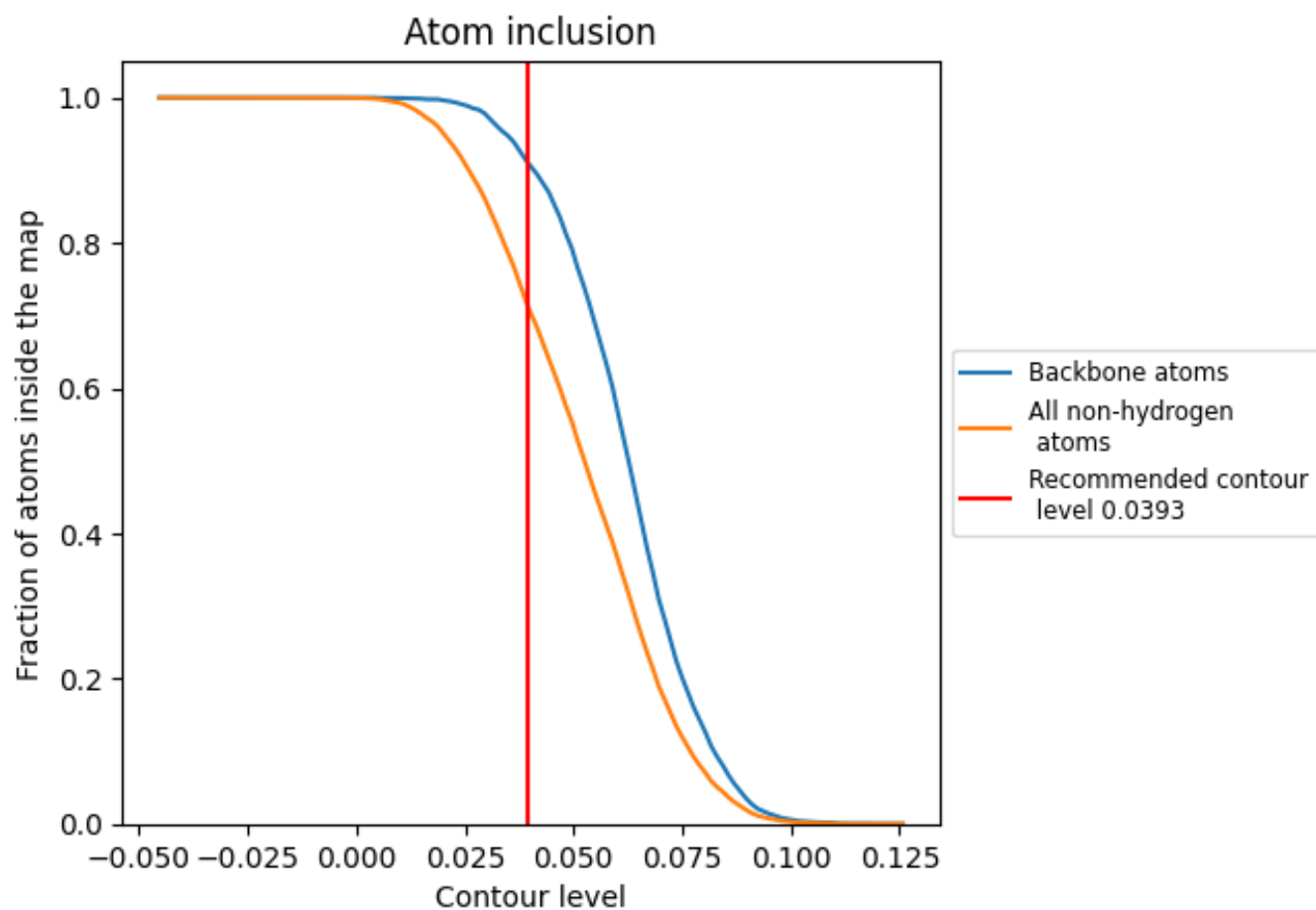
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0393).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 72% 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 (0.0393) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.3130
A	 0.7121	 0.3260
B	 0.7138	 0.3260
C	 0.7098	 0.3250
D	 0.6216	 0.2660
E	 0.6238	 0.2650
F	 0.6271	 0.2680
G	 0.7690	 0.3280
H	 0.7771	 0.3240
I	 0.7634	 0.3270
J	 0.7667	 0.3290
K	 0.7796	 0.3250
L	 0.7758	 0.3250
M	 0.6071	 0.2750
N	 0.6393	 0.2850
O	 0.6429	 0.2930
P	 0.6393	 0.2910
Q	 0.6071	 0.2830
R	 0.6557	 0.2850

