



## Full wwPDB EM Validation Report ⓘ

Sep 5, 2024 – 11:17 AM EDT

PDB ID : 8TXU  
EMDB ID : EMD-41705  
Title : Fab 3864-10 in complex with influenza HA H3-SING16  
Authors : Morano, N.C.; Shapiro, L.  
Deposited on : 2023-08-24  
Resolution : 3.22 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

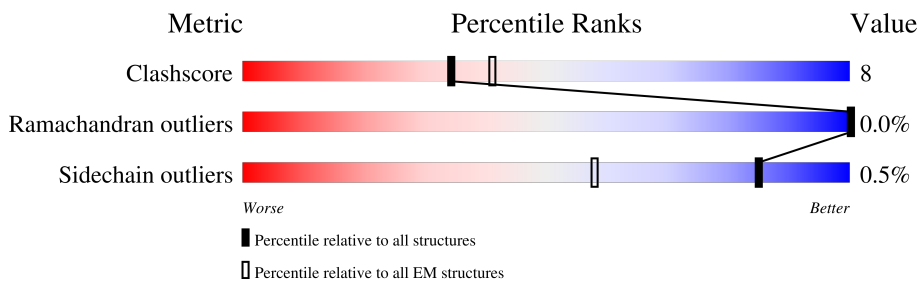
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.22 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	350	
1	C	350	
1	G	350	
2	B	232	
2	D	232	
2	I	232	
3	E	231	
3	F	231	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	231	
4	J	214	
4	K	214	
4	L	214	
5	N	5	
5	O	5	
5	R	5	
5	S	5	
5	V	5	
5	W	5	
6	P	3	
6	T	3	
6	X	3	

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 17503 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 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	325	2531	1586	449	483	13	0	0
1	C	325	2531	1586	449	483	13	0	0
1	G	325	2531	1586	449	483	13	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	CYS	THR	conflict	UNP A0A5B8WNB2
A	330	ARG	-	expression tag	UNP A0A5B8WNB2
A	331	ARG	-	expression tag	UNP A0A5B8WNB2
A	332	ARG	-	expression tag	UNP A0A5B8WNB2
A	333	ARG	-	expression tag	UNP A0A5B8WNB2
A	334	ARG	-	expression tag	UNP A0A5B8WNB2
C	30	CYS	THR	conflict	UNP A0A5B8WNB2
C	330	ARG	-	expression tag	UNP A0A5B8WNB2
C	331	ARG	-	expression tag	UNP A0A5B8WNB2
C	332	ARG	-	expression tag	UNP A0A5B8WNB2
C	333	ARG	-	expression tag	UNP A0A5B8WNB2
C	334	ARG	-	expression tag	UNP A0A5B8WNB2
G	30	CYS	THR	conflict	UNP A0A5B8WNB2
G	330	ARG	-	expression tag	UNP A0A5B8WNB2
G	331	ARG	-	expression tag	UNP A0A5B8WNB2
G	332	ARG	-	expression tag	UNP A0A5B8WNB2
G	333	ARG	-	expression tag	UNP A0A5B8WNB2
G	334	ARG	-	expression tag	UNP A0A5B8WNB2

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	168	Total	C	N	O	S	0	0
			1358	844	237	271	6		
2	D	168	Total	C	N	O	S	0	0
			1358	844	237	271	6		
2	I	168	Total	C	N	O	S	0	0
			1358	844	237	271	6		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	178	GLY	LEU	conflict	UNP A0A5B8WKM0
B	180	LEU	-	expression tag	UNP A0A5B8WKM0
B	181	VAL	-	expression tag	UNP A0A5B8WKM0
B	182	PRO	-	expression tag	UNP A0A5B8WKM0
B	183	ARG	-	expression tag	UNP A0A5B8WKM0
B	184	GLY	-	expression tag	UNP A0A5B8WKM0
B	185	SER	-	expression tag	UNP A0A5B8WKM0
B	186	PRO	-	expression tag	UNP A0A5B8WKM0
B	187	GLY	-	expression tag	UNP A0A5B8WKM0
B	188	SER	-	expression tag	UNP A0A5B8WKM0
B	189	GLY	-	expression tag	UNP A0A5B8WKM0
B	190	TYR	-	expression tag	UNP A0A5B8WKM0
B	191	ILE	-	expression tag	UNP A0A5B8WKM0
B	192	PRO	-	expression tag	UNP A0A5B8WKM0
B	193	GLU	-	expression tag	UNP A0A5B8WKM0
B	194	ALA	-	expression tag	UNP A0A5B8WKM0
B	195	PRO	-	expression tag	UNP A0A5B8WKM0
B	196	ARG	-	expression tag	UNP A0A5B8WKM0
B	197	ASP	-	expression tag	UNP A0A5B8WKM0
B	198	GLY	-	expression tag	UNP A0A5B8WKM0
B	199	GLN	-	expression tag	UNP A0A5B8WKM0
B	200	ALA	-	expression tag	UNP A0A5B8WKM0
B	201	TYR	-	expression tag	UNP A0A5B8WKM0
B	202	VAL	-	expression tag	UNP A0A5B8WKM0
B	203	ARG	-	expression tag	UNP A0A5B8WKM0
B	204	LYS	-	expression tag	UNP A0A5B8WKM0
B	205	ASP	-	expression tag	UNP A0A5B8WKM0
B	206	GLY	-	expression tag	UNP A0A5B8WKM0
B	207	GLU	-	expression tag	UNP A0A5B8WKM0
B	208	TRP	-	expression tag	UNP A0A5B8WKM0
B	209	VAL	-	expression tag	UNP A0A5B8WKM0
B	210	LEU	-	expression tag	UNP A0A5B8WKM0
B	211	LEU	-	expression tag	UNP A0A5B8WKM0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	212	SER	-	expression tag	UNP A0A5B8WKM0
B	213	THR	-	expression tag	UNP A0A5B8WKM0
B	214	PHE	-	expression tag	UNP A0A5B8WKM0
B	215	LEU	-	expression tag	UNP A0A5B8WKM0
B	216	GLY	-	expression tag	UNP A0A5B8WKM0
B	217	HIS	-	expression tag	UNP A0A5B8WKM0
B	218	HIS	-	expression tag	UNP A0A5B8WKM0
B	219	HIS	-	expression tag	UNP A0A5B8WKM0
B	220	HIS	-	expression tag	UNP A0A5B8WKM0
B	221	HIS	-	expression tag	UNP A0A5B8WKM0
B	222	HIS	-	expression tag	UNP A0A5B8WKM0
B	223	ALA	-	expression tag	UNP A0A5B8WKM0
B	224	SER	-	expression tag	UNP A0A5B8WKM0
B	225	TRP	-	expression tag	UNP A0A5B8WKM0
B	226	SER	-	expression tag	UNP A0A5B8WKM0
B	227	HIS	-	expression tag	UNP A0A5B8WKM0
B	228	PRO	-	expression tag	UNP A0A5B8WKM0
B	229	GLN	-	expression tag	UNP A0A5B8WKM0
B	230	PHE	-	expression tag	UNP A0A5B8WKM0
B	231	GLU	-	expression tag	UNP A0A5B8WKM0
B	232	LYS	-	expression tag	UNP A0A5B8WKM0
D	178	GLY	LEU	conflict	UNP A0A5B8WKM0
D	180	LEU	-	expression tag	UNP A0A5B8WKM0
D	181	VAL	-	expression tag	UNP A0A5B8WKM0
D	182	PRO	-	expression tag	UNP A0A5B8WKM0
D	183	ARG	-	expression tag	UNP A0A5B8WKM0
D	184	GLY	-	expression tag	UNP A0A5B8WKM0
D	185	SER	-	expression tag	UNP A0A5B8WKM0
D	186	PRO	-	expression tag	UNP A0A5B8WKM0
D	187	GLY	-	expression tag	UNP A0A5B8WKM0
D	188	SER	-	expression tag	UNP A0A5B8WKM0
D	189	GLY	-	expression tag	UNP A0A5B8WKM0
D	190	TYR	-	expression tag	UNP A0A5B8WKM0
D	191	ILE	-	expression tag	UNP A0A5B8WKM0
D	192	PRO	-	expression tag	UNP A0A5B8WKM0
D	193	GLU	-	expression tag	UNP A0A5B8WKM0
D	194	ALA	-	expression tag	UNP A0A5B8WKM0
D	195	PRO	-	expression tag	UNP A0A5B8WKM0
D	196	ARG	-	expression tag	UNP A0A5B8WKM0
D	197	ASP	-	expression tag	UNP A0A5B8WKM0
D	198	GLY	-	expression tag	UNP A0A5B8WKM0
D	199	GLN	-	expression tag	UNP A0A5B8WKM0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	200	ALA	-	expression tag	UNP A0A5B8WKM0
D	201	TYR	-	expression tag	UNP A0A5B8WKM0
D	202	VAL	-	expression tag	UNP A0A5B8WKM0
D	203	ARG	-	expression tag	UNP A0A5B8WKM0
D	204	LYS	-	expression tag	UNP A0A5B8WKM0
D	205	ASP	-	expression tag	UNP A0A5B8WKM0
D	206	GLY	-	expression tag	UNP A0A5B8WKM0
D	207	GLU	-	expression tag	UNP A0A5B8WKM0
D	208	TRP	-	expression tag	UNP A0A5B8WKM0
D	209	VAL	-	expression tag	UNP A0A5B8WKM0
D	210	LEU	-	expression tag	UNP A0A5B8WKM0
D	211	LEU	-	expression tag	UNP A0A5B8WKM0
D	212	SER	-	expression tag	UNP A0A5B8WKM0
D	213	THR	-	expression tag	UNP A0A5B8WKM0
D	214	PHE	-	expression tag	UNP A0A5B8WKM0
D	215	LEU	-	expression tag	UNP A0A5B8WKM0
D	216	GLY	-	expression tag	UNP A0A5B8WKM0
D	217	HIS	-	expression tag	UNP A0A5B8WKM0
D	218	HIS	-	expression tag	UNP A0A5B8WKM0
D	219	HIS	-	expression tag	UNP A0A5B8WKM0
D	220	HIS	-	expression tag	UNP A0A5B8WKM0
D	221	HIS	-	expression tag	UNP A0A5B8WKM0
D	222	HIS	-	expression tag	UNP A0A5B8WKM0
D	223	ALA	-	expression tag	UNP A0A5B8WKM0
D	224	SER	-	expression tag	UNP A0A5B8WKM0
D	225	TRP	-	expression tag	UNP A0A5B8WKM0
D	226	SER	-	expression tag	UNP A0A5B8WKM0
D	227	HIS	-	expression tag	UNP A0A5B8WKM0
D	228	PRO	-	expression tag	UNP A0A5B8WKM0
D	229	GLN	-	expression tag	UNP A0A5B8WKM0
D	230	PHE	-	expression tag	UNP A0A5B8WKM0
D	231	GLU	-	expression tag	UNP A0A5B8WKM0
D	232	LYS	-	expression tag	UNP A0A5B8WKM0
I	178	GLY	LEU	conflict	UNP A0A5B8WKM0
I	180	LEU	-	expression tag	UNP A0A5B8WKM0
I	181	VAL	-	expression tag	UNP A0A5B8WKM0
I	182	PRO	-	expression tag	UNP A0A5B8WKM0
I	183	ARG	-	expression tag	UNP A0A5B8WKM0
I	184	GLY	-	expression tag	UNP A0A5B8WKM0
I	185	SER	-	expression tag	UNP A0A5B8WKM0
I	186	PRO	-	expression tag	UNP A0A5B8WKM0
I	187	GLY	-	expression tag	UNP A0A5B8WKM0

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	188	SER	-	expression tag	UNP A0A5B8WKM0
I	189	GLY	-	expression tag	UNP A0A5B8WKM0
I	190	TYR	-	expression tag	UNP A0A5B8WKM0
I	191	ILE	-	expression tag	UNP A0A5B8WKM0
I	192	PRO	-	expression tag	UNP A0A5B8WKM0
I	193	GLU	-	expression tag	UNP A0A5B8WKM0
I	194	ALA	-	expression tag	UNP A0A5B8WKM0
I	195	PRO	-	expression tag	UNP A0A5B8WKM0
I	196	ARG	-	expression tag	UNP A0A5B8WKM0
I	197	ASP	-	expression tag	UNP A0A5B8WKM0
I	198	GLY	-	expression tag	UNP A0A5B8WKM0
I	199	GLN	-	expression tag	UNP A0A5B8WKM0
I	200	ALA	-	expression tag	UNP A0A5B8WKM0
I	201	TYR	-	expression tag	UNP A0A5B8WKM0
I	202	VAL	-	expression tag	UNP A0A5B8WKM0
I	203	ARG	-	expression tag	UNP A0A5B8WKM0
I	204	LYS	-	expression tag	UNP A0A5B8WKM0
I	205	ASP	-	expression tag	UNP A0A5B8WKM0
I	206	GLY	-	expression tag	UNP A0A5B8WKM0
I	207	GLU	-	expression tag	UNP A0A5B8WKM0
I	208	TRP	-	expression tag	UNP A0A5B8WKM0
I	209	VAL	-	expression tag	UNP A0A5B8WKM0
I	210	LEU	-	expression tag	UNP A0A5B8WKM0
I	211	LEU	-	expression tag	UNP A0A5B8WKM0
I	212	SER	-	expression tag	UNP A0A5B8WKM0
I	213	THR	-	expression tag	UNP A0A5B8WKM0
I	214	PHE	-	expression tag	UNP A0A5B8WKM0
I	215	LEU	-	expression tag	UNP A0A5B8WKM0
I	216	GLY	-	expression tag	UNP A0A5B8WKM0
I	217	HIS	-	expression tag	UNP A0A5B8WKM0
I	218	HIS	-	expression tag	UNP A0A5B8WKM0
I	219	HIS	-	expression tag	UNP A0A5B8WKM0
I	220	HIS	-	expression tag	UNP A0A5B8WKM0
I	221	HIS	-	expression tag	UNP A0A5B8WKM0
I	222	HIS	-	expression tag	UNP A0A5B8WKM0
I	223	ALA	-	expression tag	UNP A0A5B8WKM0
I	224	SER	-	expression tag	UNP A0A5B8WKM0
I	225	TRP	-	expression tag	UNP A0A5B8WKM0
I	226	SER	-	expression tag	UNP A0A5B8WKM0
I	227	HIS	-	expression tag	UNP A0A5B8WKM0
I	228	PRO	-	expression tag	UNP A0A5B8WKM0
I	229	GLN	-	expression tag	UNP A0A5B8WKM0

*Continued on next page...*



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	230	PHE	-	expression tag	UNP A0A5B8WKM0
I	231	GLU	-	expression tag	UNP A0A5B8WKM0
I	232	LYS	-	expression tag	UNP A0A5B8WKM0

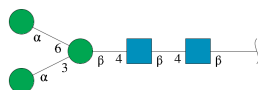
- Molecule 3 is a protein called Fab 3864-10 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	121	Total	C	N	O	S	0	0
			938	594	153	186	5		
3	F	121	Total	C	N	O	S	0	0
			938	594	153	186	5		
3	H	121	Total	C	N	O	S	0	0
			938	594	153	186	5		

- Molecule 4 is a protein called Fab 3864-10 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	107	Total	C	N	O	S	0	0
			823	509	141	169	4		
4	K	107	Total	C	N	O	S	0	0
			823	509	141	169	4		
4	L	107	Total	C	N	O	S	0	0
			823	509	141	169	4		

- Molecule 5 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.



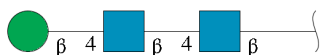
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	N	5	Total	C	N	O	0	0
			61	34	2	25		
5	O	5	Total	C	N	O	0	0
			61	34	2	25		
5	R	5	Total	C	N	O	0	0
			61	34	2	25		
5	S	5	Total	C	N	O	0	0
			61	34	2	25		

Continued on next page...

Continued from previous page...

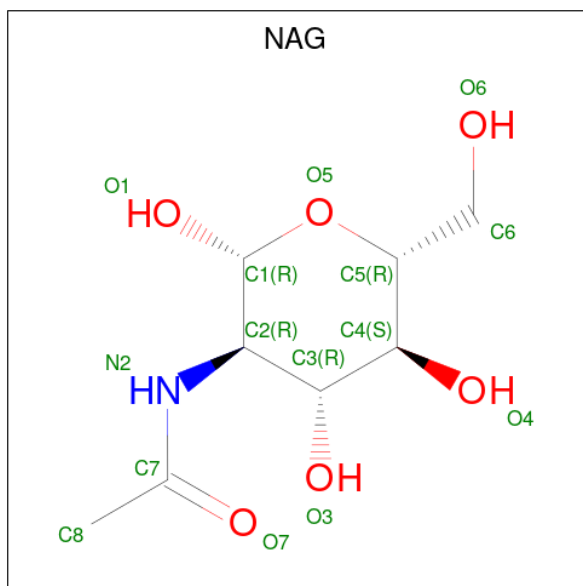
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	V	5	61	34	2	25	0	0
5	W	5	61	34	2	25	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	P	3	39	22	2	15	0	0
6	T	3	39	22	2	15	0	0
6	X	3	39	22	2	15	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	14	8	1	5	0

Continued on next page...

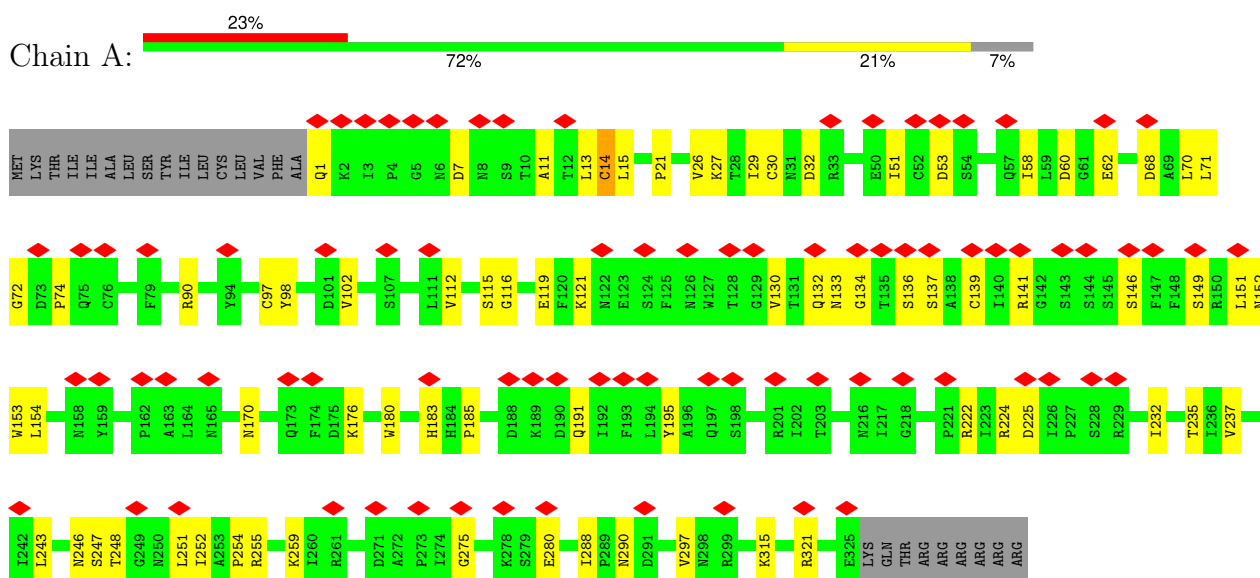
*Continued from previous page...*

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

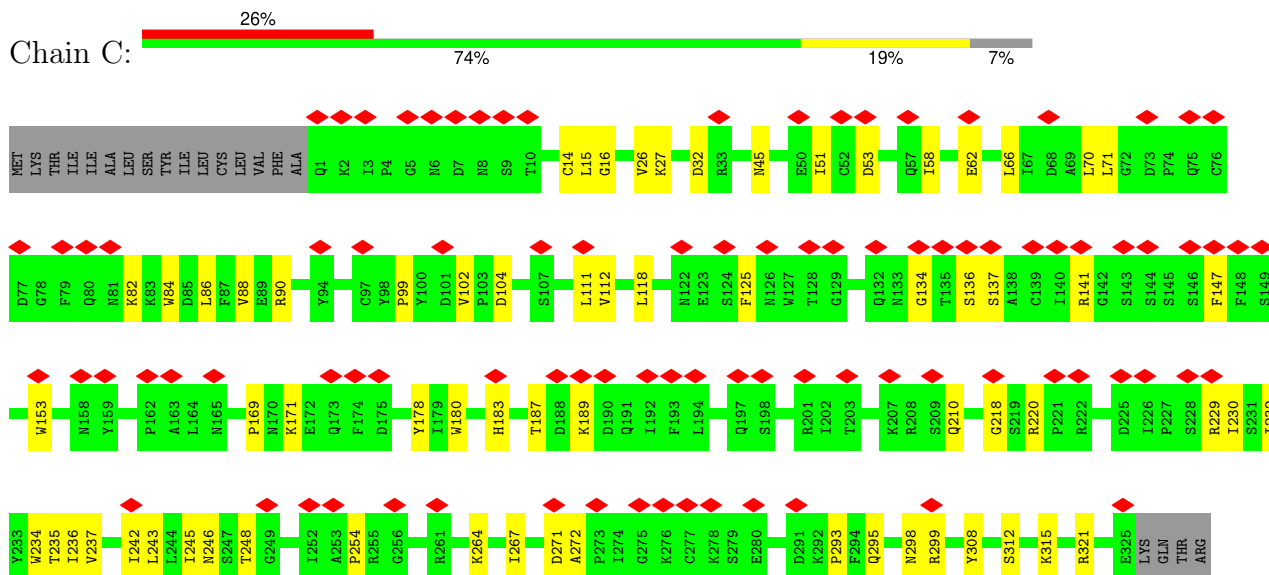
### 3 Residue-property plots [i](#)

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

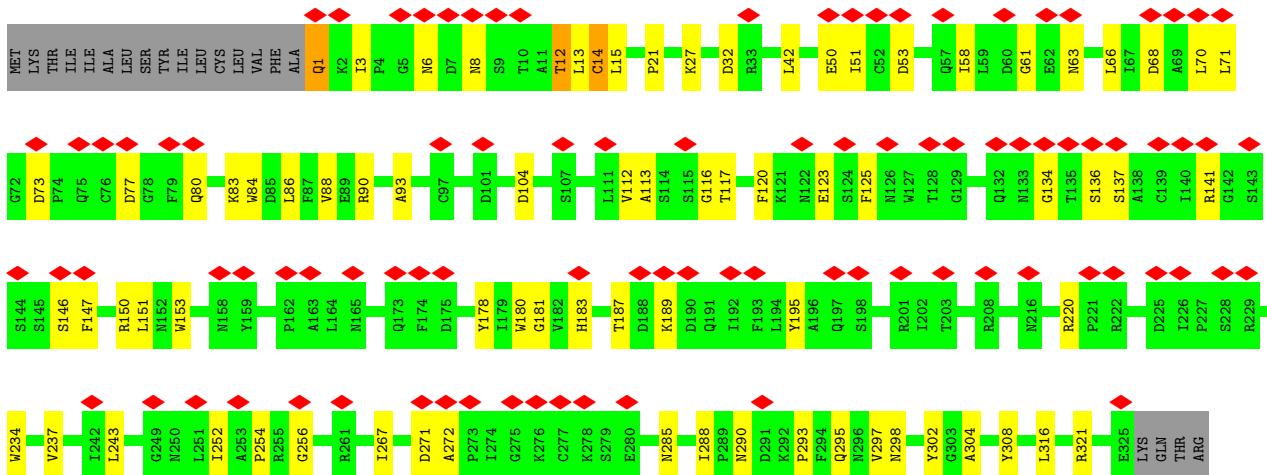


- Molecule 1: Hemagglutinin HA1 chain



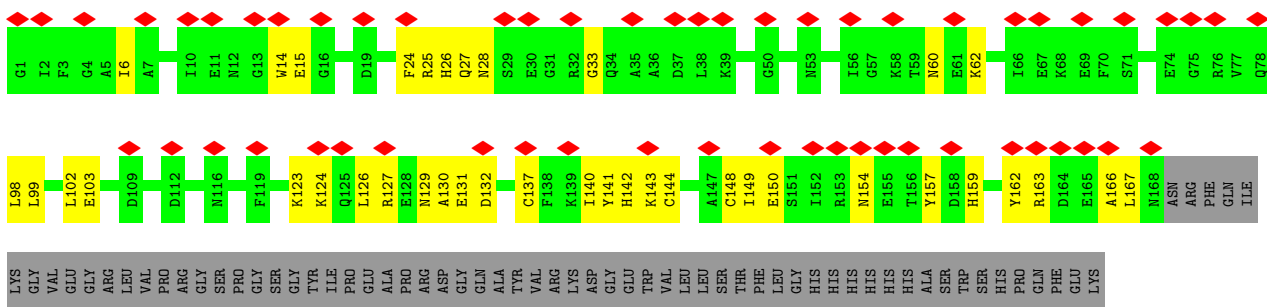
ARG  
ARG  
ARG  
ARG

• Molecule 1: Hemagglutinin HA1 chain

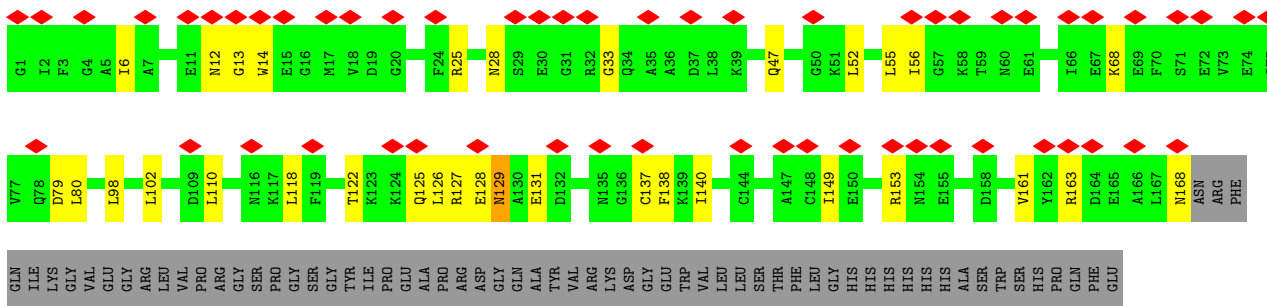


ARG  
ARG  
ARG  
ARG

• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

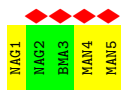




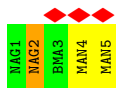
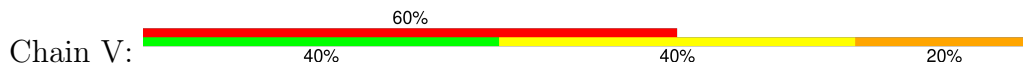




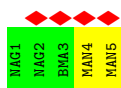




- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 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, Not provided	
Number of particles used	90799	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.06	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.595	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.164	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: NAG, BMA, MAN

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	0/2589	0.59	0/3518
1	C	0.30	0/2589	0.59	0/3518
1	G	0.32	0/2589	0.60	0/3518
2	B	0.30	0/1381	0.60	0/1855
2	D	0.33	0/1381	0.63	0/1855
2	I	0.29	0/1381	0.58	0/1855
3	E	0.28	0/962	0.53	0/1304
3	F	0.29	0/962	0.56	0/1304
3	H	0.29	0/962	0.54	0/1304
4	J	0.26	0/836	0.55	0/1131
4	K	0.25	0/836	0.55	0/1131
4	L	0.26	0/836	0.56	0/1131
All	All	0.30	0/17304	0.58	0/23424

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	2531	0	2492	58	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2531	0	2495	44	0
1	G	2531	0	2495	63	0
2	B	1358	0	1287	31	0
2	D	1358	0	1288	26	0
2	I	1358	0	1288	31	0
3	E	938	0	892	7	0
3	F	938	0	892	10	0
3	H	938	0	892	11	0
4	J	823	0	805	12	0
4	K	823	0	805	7	0
4	L	823	0	805	9	0
5	N	61	0	52	0	0
5	O	61	0	52	2	0
5	R	61	0	52	0	0
5	S	61	0	52	2	0
5	V	61	0	52	1	0
5	W	61	0	52	0	0
6	P	39	0	34	0	0
6	T	39	0	34	0	0
6	X	39	0	34	0	0
7	A	56	0	52	0	0
7	B	14	0	13	0	0
All	All	17503	0	16915	273	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 (273) 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:G:8:ASN:ND2	1:G:12:THR:CB	2.01	1.23
1:G:8:ASN:ND2	1:G:12:THR:HG21	1.53	1.22
1:G:8:ASN:ND2	1:G:12:THR:OG1	1.73	1.21
1:G:8:ASN:ND2	1:G:12:THR:CG2	2.05	1.19
1:A:13:LEU:HD12	2:B:140:ILE:HD12	1.22	1.16
1:G:8:ASN:HD21	1:G:12:THR:HG21	1.17	0.92
1:G:8:ASN:CG	1:G:12:THR:HG21	1.96	0.86
2:B:150:GLU:O	2:B:154:ASN:HB2	1.77	0.84
1:G:8:ASN:HD21	1:G:12:THR:CG2	1.75	0.84
1:G:8:ASN:HD22	1:G:12:THR:HG1	1.21	0.83
1:A:70:LEU:HD11	1:A:112:VAL:HG11	1.64	0.80

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:CYS:HA	2:B:137:CYS:HA	1.65	0.78
2:B:127:ARG:HD2	2:D:131:GLU:HB2	1.66	0.77
1:G:8:ASN:HD22	1:G:12:THR:CB	1.85	0.72
1:A:13:LEU:CD1	2:B:140:ILE:HD12	2.13	0.71
2:I:33:GLY:HA2	3:F:102:GLY:HA3	1.73	0.70
3:H:62:GLN:O	3:H:65:LYS:NZ	2.26	0.69
4:L:34:ASN:HD22	4:L:89:GLN:HE21	1.39	0.68
1:A:13:LEU:HD13	2:B:149:ILE:CD1	2.25	0.66
1:C:14:CYS:SG	1:C:15:LEU:N	2.69	0.66
1:G:8:ASN:HD21	1:G:12:THR:CB	1.93	0.65
2:I:142:HIS:HD1	2:I:157:TYR:HH	1.44	0.64
1:G:141:ARG:NH2	1:G:147:PHE:O	2.31	0.63
3:F:30:ILE:HA	3:F:53:PRO:HB2	1.79	0.63
1:A:72:GLY:HA3	1:A:149:SER:H	1.63	0.63
1:A:13:LEU:HD12	2:B:140:ILE:CD1	2.14	0.63
2:B:123:LYS:NZ	2:B:132:ASP:OD2	2.32	0.63
4:L:33:LEU:HD11	4:L:88:CYS:HB2	1.81	0.63
1:A:180:TRP:HB3	1:A:254:PRO:HD3	1.81	0.62
2:D:47:GLN:OE1	2:D:110:LEU:HD13	1.99	0.62
2:I:35:ALA:HB1	2:I:153:ARG:HD3	1.80	0.62
1:G:14:CYS:SG	1:G:15:LEU:N	2.74	0.61
1:A:133:ASN:OD1	1:A:255:ARG:NH1	2.33	0.61
1:G:68:ASP:HB3	1:G:73:ASP:HB2	1.83	0.61
1:G:13:LEU:HD22	2:I:26:HIS:HB2	1.82	0.61
1:C:70:LEU:HD11	1:C:112:VAL:HG11	1.82	0.60
3:F:20:LEU:HB2	3:F:81:MET:HB2	1.83	0.60
1:G:104:ASP:HB3	1:G:234:TRP:HH2	1.67	0.60
4:K:34:ASN:HB2	4:K:89:GLN:HB3	1.82	0.60
1:G:58:ILE:HG12	1:G:86:LEU:HB3	1.84	0.59
1:A:280:GLU:OE2	1:A:290:ASN:ND2	2.35	0.59
1:G:13:LEU:HD21	2:I:149:ILE:HD11	1.84	0.59
2:B:33:GLY:HA2	3:H:102:GLY:HA3	1.85	0.59
3:E:30:ILE:HA	3:E:53:PRO:HB2	1.85	0.58
1:A:153:TRP:NE1	1:A:195:TYR:OH	2.37	0.58
2:D:12:ASN:ND2	2:D:13:GLY:O	2.37	0.58
1:A:288:ILE:HG21	1:A:297:VAL:HG21	1.85	0.57
1:G:136:SER:OG	1:G:137:SER:N	2.37	0.57
1:A:170:ASN:HD22	1:A:237:VAL:HG12	1.68	0.57
1:A:170:ASN:OD1	1:A:176:LYS:NZ	2.37	0.57
1:G:80:GLN:OE1	1:G:150:ARG:NH1	2.37	0.57
2:B:60:ASN:HB3	2:B:62:LYS:HE3	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLY:HA3	2:D:25:ARG:HD2	1.87	0.57
3:H:33:TRP:NE1	3:H:52:ASP:OD1	2.37	0.57
2:I:14:TRP:H	2:I:25:ARG:HH22	1.53	0.57
3:E:62:GLN:O	3:E:65:LYS:NZ	2.32	0.57
1:A:11:ALA:HB1	1:A:13:LEU:HD21	1.86	0.57
1:C:15:LEU:HD22	2:D:118:LEU:HD23	1.87	0.57
1:C:66:LEU:HD13	1:C:267:ILE:HD12	1.87	0.56
1:G:290:ASN:ND2	1:G:304:ALA:O	2.38	0.56
2:B:163:ARG:HD2	2:D:168:ASN:HD22	1.71	0.56
1:C:141:ARG:NH2	1:C:147:PHE:O	2.39	0.56
1:G:141:ARG:HE	1:G:146:SER:HB3	1.71	0.56
3:H:30:ILE:HA	3:H:53:PRO:HB2	1.86	0.56
1:C:104:ASP:HB3	1:C:234:TRP:HH2	1.71	0.56
1:C:26:VAL:HG12	1:C:315:LYS:HB2	1.87	0.56
1:C:187:THR:HG22	1:C:189:LYS:H	1.71	0.55
1:C:62:GLU:HA	1:C:90:ARG:HG3	1.88	0.55
1:G:321:ARG:HB3	2:I:6:ILE:HD12	1.87	0.55
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.88	0.55
2:D:33:GLY:HA2	3:E:102:GLY:HA3	1.88	0.55
1:G:8:ASN:ND2	1:G:12:THR:HB	2.16	0.55
1:G:71:LEU:HD13	1:G:151:LEU:HD21	1.88	0.55
1:A:26:VAL:HG12	1:A:315:LYS:HB2	1.88	0.55
2:I:34:GLN:NE2	3:F:104:SER:OG	2.39	0.55
1:A:180:TRP:HE1	1:A:235:THR:HG1	1.55	0.54
2:I:129:ASN:HB3	2:I:162:TYR:HB3	1.88	0.54
1:G:66:LEU:HD13	1:G:267:ILE:HD12	1.89	0.54
1:G:187:THR:HG22	1:G:189:LYS:H	1.71	0.54
1:A:68:ASP:HA	1:A:71:LEU:HB2	1.90	0.54
2:B:129:ASN:HB3	2:B:162:TYR:HB3	1.90	0.54
1:C:293:PRO:HG3	2:D:55:LEU:HB3	1.89	0.54
4:J:39:LYS:NZ	4:J:81:GLU:O	2.41	0.54
2:B:126:LEU:HD11	2:B:141:TYR:H	1.73	0.54
4:K:37:GLN:HB2	4:K:47:LEU:HD11	1.90	0.54
1:G:6:ASN:HB2	3:F:57:TYR:HE1	1.73	0.53
1:A:132:GLN:HB3	1:A:152:ASN:HD21	1.73	0.53
1:A:13:LEU:HD23	2:B:27:GLN:H	1.73	0.53
1:C:180:TRP:HE1	1:C:235:THR:HG1	1.56	0.53
2:B:131:GLU:HG2	2:B:167:LEU:HD21	1.91	0.53
1:G:180:TRP:HB3	1:G:254:PRO:HD3	1.90	0.53
1:G:237:VAL:HG21	1:G:243:LEU:HB2	1.90	0.53
1:C:295:GLN:NE2	1:C:298:ASN:O	2.41	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLN:OE1	1:G:220:ARG:NE	2.43	0.52
1:A:51:ILE:O	1:A:275:GLY:N	2.38	0.52
1:A:27:LYS:HG3	1:A:32:ASP:HA	1.92	0.52
1:C:45:ASN:ND2	1:C:312:SER:O	2.42	0.52
1:G:8:ASN:CG	1:G:12:THR:CG2	2.67	0.52
1:A:119:GLU:HB2	1:A:259:LYS:HB2	1.92	0.52
1:G:304:ALA:HB2	2:I:61:GLU:HG3	1.92	0.51
1:A:119:GLU:HB3	1:A:121:LYS:HE3	1.92	0.51
1:A:134:GLY:HA3	1:A:153:TRP:HE3	1.75	0.51
1:A:321:ARG:HB3	2:B:6:ILE:HD12	1.92	0.51
1:G:51:ILE:HD13	1:G:88:VAL:HG11	1.91	0.51
1:A:222:ARG:NH1	5:V:2:NAG:O6	2.44	0.51
3:E:69:ARG:HB3	3:E:82:GLN:HB3	1.92	0.51
1:G:120:PHE:HD1	1:G:150:ARG:HE	1.57	0.51
3:F:34:MET:HB2	3:F:51:ILE:HG22	1.93	0.51
1:A:60:ASP:OD1	1:A:90:ARG:NH2	2.44	0.51
1:G:21:PRO:HD3	2:I:15:GLU:HB3	1.92	0.51
1:A:70:LEU:HD21	1:A:112:VAL:HG21	1.93	0.50
1:C:218:GLY:H	1:C:220:ARG:HH12	1.57	0.50
4:J:61:ARG:NH2	4:J:81:GLU:OE2	2.44	0.50
1:A:170:ASN:CG	1:A:176:LYS:HZ3	2.15	0.50
2:I:24:PHE:H	2:I:35:ALA:HB3	1.75	0.50
2:I:91:LEU:O	2:I:95:ASN:HB2	2.12	0.50
2:D:14:TRP:HB2	2:D:25:ARG:HE	1.75	0.50
1:C:271:ASP:OD1	1:C:271:ASP:N	2.44	0.50
3:F:35:HIS:CD2	3:F:99:GLY:HA3	2.47	0.50
1:C:134:GLY:HA3	1:C:153:TRP:HE3	1.76	0.50
3:F:98:ARG:NH2	3:F:108:ASP:OD2	2.38	0.50
1:C:90:ARG:NH2	1:C:272:ALA:O	2.45	0.49
2:I:38:LEU:O	2:I:42:GLN:HB2	2.11	0.49
3:H:40:ARG:HB2	3:H:43:GLN:HB2	1.93	0.49
1:G:8:ASN:OD1	1:G:12:THR:HG21	2.12	0.49
1:A:21:PRO:HD3	2:B:15:GLU:HB3	1.94	0.49
2:D:122:THR:HG22	2:D:126:LEU:HG	1.92	0.49
1:A:185:PRO:HG2	1:A:191:GLN:HB2	1.93	0.49
2:I:120:GLU:HA	2:I:123:LYS:HG2	1.93	0.49
4:K:39:LYS:NZ	4:K:81:GLU:O	2.46	0.49
2:D:129:ASN:O	2:D:129:ASN:ND2	2.37	0.49
1:G:271:ASP:OD1	1:G:271:ASP:N	2.43	0.49
2:I:142:HIS:ND1	2:I:157:TYR:OH	2.36	0.49
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:39:LYS:NZ	4:L:81:GLU:O	2.45	0.49
1:G:83:LYS:HG2	1:G:117:THR:HG23	1.93	0.48
2:B:132:ASP:OD1	2:B:132:ASP:N	2.44	0.48
1:C:70:LEU:HD21	1:C:112:VAL:HG21	1.96	0.48
2:D:137:CYS:SG	2:D:138:PHE:N	2.86	0.48
1:G:27:LYS:HG3	1:G:32:ASP:HA	1.95	0.48
1:G:134:GLY:HA3	1:G:153:TRP:HE3	1.77	0.48
1:A:136:SER:OG	1:A:137:SER:N	2.47	0.48
2:B:142:HIS:ND1	2:B:157:TYR:OH	2.47	0.48
1:C:299:ARG:HB3	2:D:68:LYS:HD3	1.96	0.48
1:G:1:GLN:HA	1:G:1:GLN:HE21	1.79	0.48
2:B:99:LEU:O	2:B:103:GLU:HG2	2.14	0.48
1:C:27:LYS:HG3	1:C:32:ASP:HA	1.96	0.48
1:C:99:PRO:HB2	1:C:229:ARG:HD3	1.96	0.48
2:D:14:TRP:HB2	2:D:25:ARG:HH21	1.78	0.47
1:G:293:PRO:HG3	2:I:55:LEU:HB3	1.95	0.47
1:G:153:TRP:NE1	1:G:195:TYR:OH	2.42	0.47
1:A:224:ARG:O	1:A:225:ASP:HB2	2.14	0.47
2:B:14:TRP:HB2	2:B:25:ARG:HH21	1.79	0.47
1:A:246:ASN:HD21	5:O:1:NAG:HN2	1.61	0.47
1:C:51:ILE:HD13	1:C:88:VAL:HG11	1.97	0.47
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.95	0.47
1:C:180:TRP:HB3	1:C:254:PRO:HD3	1.97	0.47
4:J:30:SER:O	4:J:71:TYR:OH	2.31	0.47
3:H:39:GLN:NE2	4:L:38:GLN:OE1	2.35	0.47
1:C:169:PRO:HB2	1:C:171:LYS:HE3	1.96	0.47
1:A:13:LEU:CD2	2:B:27:GLN:H	2.28	0.46
1:A:62:GLU:HA	1:A:90:ARG:HG3	1.97	0.46
2:D:125:GLN:HA	2:D:161:VAL:HG22	1.97	0.46
1:G:288:ILE:HG21	1:G:297:VAL:HG21	1.96	0.46
4:L:61:ARG:NH2	4:L:81:GLU:OE2	2.45	0.46
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.98	0.46
2:D:128:GLU:HB3	2:D:161:VAL:HG11	1.97	0.46
1:A:1:GLN:NE2	1:A:14:CYS:SG	2.88	0.46
1:C:53:ASP:OD1	1:C:53:ASP:N	2.48	0.46
1:C:321:ARG:HB3	2:D:6:ILE:HD12	1.97	0.46
1:G:125:PHE:HZ	1:G:178:TYR:HE2	1.64	0.46
3:E:40:ARG:HB2	3:E:43:GLN:HB2	1.97	0.46
1:A:130:VAL:HG11	1:A:154:LEU:HD23	1.98	0.46
1:C:169:PRO:HB3	1:C:242:ILE:HG12	1.97	0.46
2:D:52:LEU:O	2:D:56:ILE:N	2.44	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:66:GLY:O	3:H:84:SER:OG	2.34	0.46
4:L:37:GLN:HG2	4:L:47:LEU:HD11	1.98	0.46
1:A:1:GLN:HB3	1:A:14:CYS:SG	2.56	0.46
1:A:11:ALA:O	1:A:13:LEU:HG	2.16	0.46
1:C:136:SER:HB2	1:C:147:PHE:HD1	1.80	0.45
1:C:246:ASN:HD21	5:S:1:NAG:HN2	1.64	0.45
2:D:79:ASP:OD1	2:D:80:LEU:N	2.50	0.45
3:H:103:SER:HA	4:L:96:ARG:HH22	1.80	0.45
1:G:295:GLN:HG2	1:G:308:TYR:HA	1.98	0.45
4:J:20:THR:HG22	4:J:74:THR:HG23	1.99	0.45
4:L:34:ASN:HB2	4:L:89:GLN:HG2	1.99	0.45
4:L:20:THR:HG22	4:L:74:THR:HG23	1.97	0.45
1:A:97:CYS:SG	1:A:98:TYR:N	2.89	0.45
2:I:133:MET:HG3	2:I:139:LYS:HB3	1.99	0.45
2:B:123:LYS:O	2:B:127:ARG:HG3	2.17	0.45
4:J:4:MET:SD	4:J:90:GLN:HB3	2.57	0.45
3:F:23:LYS:HE2	3:F:23:LYS:HB2	1.75	0.45
1:C:136:SER:OG	1:C:137:SER:N	2.50	0.44
2:D:28:ASN:HD21	2:D:149:ILE:HD12	1.82	0.44
4:K:35:TRP:HD1	4:K:48:ILE:HB	1.83	0.44
1:A:72:GLY:HA3	1:A:149:SER:N	2.32	0.44
2:B:127:ARG:HB3	2:D:131:GLU:HG3	1.98	0.44
1:C:84:TRP:HZ3	1:C:118:LEU:HB2	1.83	0.44
1:C:125:PHE:HZ	1:C:178:TYR:HE2	1.64	0.44
2:B:98:LEU:O	2:B:102:LEU:HG	2.18	0.44
2:I:140:ILE:HG22	2:I:142:HIS:H	1.82	0.44
1:A:183:HIS:HB2	1:A:252:ILE:HD11	2.00	0.44
2:B:26:HIS:ND1	2:B:28:ASN:OD1	2.51	0.44
1:G:285:ASN:HD22	1:G:297:VAL:HG12	1.82	0.44
1:G:181:GLY:N	1:G:252:ILE:O	2.51	0.44
2:I:124:LYS:HB2	2:I:159:HIS:CD2	2.53	0.43
3:E:103:SER:HA	4:J:96:ARG:HH22	1.83	0.43
1:C:248:THR:OG1	5:S:1:NAG:O7	2.36	0.43
2:D:126:LEU:HD21	2:D:140:ILE:HG23	2.01	0.43
2:I:15:GLU:OE2	2:I:15:GLU:N	2.51	0.43
1:A:247:SER:HB3	1:A:251:LEU:HD22	2.00	0.43
1:C:243:LEU:HD21	1:C:245:ILE:HG12	2.01	0.43
3:H:108:ASP:OD1	3:H:108:ASP:N	2.44	0.43
1:A:15:LEU:HD22	2:B:24:PHE:HD1	1.84	0.43
4:J:1:ASP:H1	4:J:95:PRO:HD2	1.83	0.43
1:A:32:ASP:OD1	1:A:32:ASP:N	2.50	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:LEU:HD11	1:G:316:LEU:HD12	2.01	0.43
1:G:84:TRP:CZ2	1:G:116:GLY:HA2	2.53	0.43
1:C:58:ILE:HG12	1:C:86:LEU:HB3	2.00	0.43
2:I:68:LYS:NZ	2:I:85:GLU:OE2	2.43	0.42
4:J:34:ASN:HB3	4:J:46:LEU:HD11	2.00	0.42
1:A:248:THR:OG1	5:O:1:NAG:O7	2.37	0.42
1:C:111:LEU:HD21	1:C:236:ILE:HD11	2.01	0.42
1:G:13:LEU:HB3	1:G:14:CYS:H	1.75	0.42
2:D:98:LEU:O	2:D:102:LEU:HG	2.19	0.42
1:G:63:ASN:HA	1:G:93:ALA:HA	2.00	0.42
1:A:30:CYS:SG	2:I:106:HIS:HE1	2.43	0.42
2:I:55:LEU:HD21	2:I:99:LEU:HD21	2.01	0.42
1:A:13:LEU:O	1:A:15:LEU:N	2.53	0.42
1:A:115:SER:OG	1:A:116:GLY:N	2.52	0.42
1:C:295:GLN:HG2	1:C:308:TYR:HA	2.02	0.42
1:G:50:GLU:HA	1:G:272:ALA:HB1	2.02	0.42
1:G:77:ASP:OD1	1:G:141:ARG:NH1	2.52	0.42
1:G:295:GLN:NE2	1:G:298:ASN:O	2.53	0.42
2:I:98:LEU:O	2:I:102:LEU:HG	2.20	0.42
1:C:71:LEU:HD21	1:C:232:ILE:HG13	2.02	0.42
2:I:14:TRP:H	2:I:25:ARG:HH12	1.68	0.42
1:A:53:ASP:HA	1:A:58:ILE:HD12	2.01	0.42
2:B:144:CYS:HB2	2:B:148:CYS:HB2	1.70	0.41
1:G:84:TRP:HH2	1:G:113:ALA:HA	1.85	0.41
2:I:123:LYS:O	2:I:127:ARG:N	2.51	0.41
4:J:37:GLN:HB2	4:J:47:LEU:HD11	2.02	0.41
1:G:123:GLU:HB3	1:G:256:GLY:HA2	2.02	0.41
2:I:58:LYS:HD3	2:I:58:LYS:HA	1.93	0.41
4:K:20:THR:HG22	4:K:74:THR:HG23	2.02	0.41
3:H:38:LYS:HB2	3:H:48:ILE:HD11	2.02	0.41
1:G:61:GLY:HA3	1:G:90:ARG:HG2	2.01	0.41
4:K:35:TRP:CZ3	4:K:88:CYS:HB3	2.55	0.41
2:I:119:PHE:HD2	2:I:138:PHE:HE2	1.68	0.41
2:I:14:TRP:CE3	2:I:25:ARG:HG2	2.56	0.41
2:B:124:LYS:HB3	2:B:159:HIS:CE1	2.56	0.41
1:G:70:LEU:HD13	1:G:112:VAL:HG11	2.02	0.41
3:F:47:TRP:HZ2	3:F:50:GLU:HB3	1.85	0.41
2:D:47:GLN:OE1	2:D:110:LEU:HD22	2.20	0.41
1:G:1:GLN:HE21	1:G:1:GLN:CA	2.34	0.41
3:H:47:TRP:HZ2	3:H:50:GLU:HB3	1.85	0.41
1:A:141:ARG:NH2	1:A:146:SER:OG	2.54	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:ARG:HH22	2:D:163:ARG:HH12	1.67	0.41
4:J:4:MET:HG2	4:J:25:ALA:HA	2.03	0.41
1:A:29:ILE:HD12	2:B:102:LEU:HD23	2.03	0.41
2:B:130:ALA:H	2:B:166:ALA:HB1	1.86	0.41
1:A:151:LEU:HB3	1:A:252:ILE:HG22	2.02	0.40
2:D:129:ASN:HD22	2:D:129:ASN:C	2.14	0.40
3:E:44:GLY:HA2	4:J:87:PHE:HE2	1.87	0.40
1:A:74:PRO:HG3	1:A:139:CYS:HA	2.02	0.40
1:C:102:VAL:HG22	1:C:232:ILE:HB	2.03	0.40
1:C:183:HIS:HA	1:C:230:ILE:HG22	2.04	0.40
1:G:86:LEU:HB2	1:G:302:TYR:CE2	2.56	0.40
1:C:82:LYS:HE2	1:C:82:LYS:HB2	1.85	0.40
2:I:68:LYS:HG2	2:I:85:GLU:HG2	2.03	0.40
4:K:61:ARG:NH2	4:K:81:GLU:OE2	2.51	0.40
1:G:53:ASP:OD1	1:G:53:ASP:N	2.54	0.40
4:J:35:TRP:CZ3	4:J:88:CYS:HB3	2.56	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	323/350 (92%)	287 (89%)	35 (11%)	1 (0%)	37	68
1	C	323/350 (92%)	288 (89%)	35 (11%)	0	100	100
1	G	323/350 (92%)	286 (88%)	37 (12%)	0	100	100
2	B	166/232 (72%)	151 (91%)	15 (9%)	0	100	100
2	D	166/232 (72%)	152 (92%)	14 (8%)	0	100	100
2	I	166/232 (72%)	154 (93%)	12 (7%)	0	100	100
3	E	119/231 (52%)	115 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	119/231 (52%)	117 (98%)	2 (2%)	0	100	100
3	H	119/231 (52%)	116 (98%)	3 (2%)	0	100	100
4	J	105/214 (49%)	99 (94%)	6 (6%)	0	100	100
4	K	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
4	L	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
All	All	2139/3081 (69%)	1965 (92%)	173 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	CYS

### 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	287/310 (93%)	286 (100%)	1 (0%)	91	95
1	C	287/310 (93%)	286 (100%)	1 (0%)	91	95
1	G	287/310 (93%)	283 (99%)	4 (1%)	62	80
2	B	143/196 (73%)	142 (99%)	1 (1%)	81	90
2	D	143/196 (73%)	141 (99%)	2 (1%)	62	80
2	I	143/196 (73%)	143 (100%)	0	100	100
3	E	101/199 (51%)	101 (100%)	0	100	100
3	F	101/199 (51%)	101 (100%)	0	100	100
3	H	101/199 (51%)	101 (100%)	0	100	100
4	J	95/194 (49%)	94 (99%)	1 (1%)	70	84
4	K	95/194 (49%)	95 (100%)	0	100	100
4	L	95/194 (49%)	95 (100%)	0	100	100
All	All	1878/2697 (70%)	1868 (100%)	10 (0%)	85	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
2	B	143	LYS
1	C	264	LYS
2	D	129	ASN
2	D	153	ARG
1	G	1	GLN
1	G	3	ILE
1	G	12	THR
1	G	14	CYS
4	J	92	ASN

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	1	GLN
2	D	12	ASN
1	G	8	ASN
2	I	34	GLN
2	I	106	HIS
4	J	92	ASN
4	L	89	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](#)

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	N	1	5	14,14,15	0.35	0	17,19,21	0.42	0
5	NAG	N	2	5	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
5	BMA	N	3	5	11,11,12	0.64	0	15,15,17	0.70	0
5	MAN	N	4	5	11,11,12	0.75	0	15,15,17	0.93	2 (13%)
5	MAN	N	5	5	11,11,12	0.72	0	15,15,17	0.97	2 (13%)
5	NAG	O	1	5	14,14,15	0.19	0	17,19,21	0.47	0
5	NAG	O	2	5	14,14,15	0.22	0	17,19,21	0.46	0
5	BMA	O	3	5	11,11,12	0.65	0	15,15,17	0.85	0
5	MAN	O	4	5	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
5	MAN	O	5	5	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
6	NAG	P	1	6	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	P	2	6	14,14,15	0.24	0	17,19,21	0.45	0
6	BMA	P	3	6	11,11,12	0.69	0	15,15,17	0.78	0
5	NAG	R	1	5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	R	2	5	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
5	BMA	R	3	5	11,11,12	0.70	0	15,15,17	0.73	0
5	MAN	R	4	5	11,11,12	0.72	0	15,15,17	1.03	2 (13%)
5	MAN	R	5	5	11,11,12	0.70	0	15,15,17	0.96	2 (13%)
5	NAG	S	1	5	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	S	2	5	14,14,15	0.24	0	17,19,21	0.47	0
5	BMA	S	3	5	11,11,12	0.68	0	15,15,17	0.82	0
5	MAN	S	4	5	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
5	MAN	S	5	5	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
6	NAG	T	1	6	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	T	2	6	14,14,15	0.23	0	17,19,21	0.43	0
6	BMA	T	3	6	11,11,12	0.67	0	15,15,17	0.78	0
5	NAG	V	1	5	14,14,15	0.37	0	17,19,21	0.40	0
5	NAG	V	2	5	14,14,15	0.39	0	17,19,21	1.02	2 (11%)
5	BMA	V	3	5	11,11,12	0.68	0	15,15,17	0.79	0
5	MAN	V	4	5	11,11,12	0.78	0	15,15,17	0.99	2 (13%)
5	MAN	V	5	5	11,11,12	0.71	0	15,15,17	0.97	2 (13%)
5	NAG	W	1	5	14,14,15	0.19	0	17,19,21	0.46	0
5	NAG	W	2	5	14,14,15	0.20	0	17,19,21	0.45	0
5	BMA	W	3	5	11,11,12	0.67	0	15,15,17	0.87	0
5	MAN	W	4	5	11,11,12	0.72	0	15,15,17	1.00	2 (13%)
5	MAN	W	5	5	11,11,12	0.74	0	15,15,17	0.95	2 (13%)
6	NAG	X	1	6	14,14,15	0.32	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	X	2	6	14,14,15	0.33	0	17,19,21	0.50	0
6	BMA	X	3	6	11,11,12	0.65	0	15,15,17	0.75	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. '2' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	W	1	5	-	1/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
5	MAN	W	4	5	-	0/2/19/22	0/1/1/1
5	MAN	W	5	5	-	0/2/19/22	0/1/1/1
6	NAG	X	1	6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	BMA	X	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	5	MAN	C1-O5-C5	2.92	116.10	112.19
5	S	5	MAN	C1-O5-C5	2.85	116.01	112.19
5	S	4	MAN	C1-O5-C5	2.73	115.85	112.19
5	R	4	MAN	C1-O5-C5	2.71	115.81	112.19
5	O	4	MAN	C1-O5-C5	2.69	115.79	112.19
5	W	4	MAN	C1-O5-C5	2.63	115.71	112.19
5	N	2	NAG	C2-N2-C7	2.56	126.33	122.90
5	R	2	NAG	C2-N2-C7	2.55	126.31	122.90
5	V	2	NAG	C2-N2-C7	2.48	126.22	122.90
5	N	5	MAN	C1-O5-C5	2.39	115.39	112.19
5	V	5	MAN	C1-O5-C5	2.38	115.38	112.19
5	V	2	NAG	C1-O5-C5	2.38	115.38	112.19
5	R	5	MAN	C1-O5-C5	2.37	115.36	112.19
5	W	5	MAN	C1-O5-C5	2.35	115.34	112.19
5	V	4	MAN	C1-O5-C5	2.30	115.27	112.19
5	S	5	MAN	O2-C2-C3	-2.18	105.63	110.15
5	O	5	MAN	O2-C2-C3	-2.17	105.65	110.15
5	V	5	MAN	O2-C2-C3	-2.14	105.71	110.15
5	N	5	MAN	O2-C2-C3	-2.12	105.76	110.15
5	W	5	MAN	O2-C2-C3	-2.11	105.78	110.15
5	V	4	MAN	O2-C2-C3	-2.10	105.79	110.15
5	O	4	MAN	O2-C2-C3	-2.10	105.80	110.15
5	R	5	MAN	O2-C2-C3	-2.09	105.82	110.15
5	N	4	MAN	C1-O5-C5	2.08	114.97	112.19
5	W	4	MAN	O2-C2-C3	-2.08	105.85	110.15
5	R	4	MAN	O2-C2-C3	-2.07	105.86	110.15
5	N	4	MAN	O2-C2-C3	-2.07	105.87	110.15
5	S	4	MAN	O2-C2-C3	-2.05	105.90	110.15

There are no chirality outliers.

All (37) torsion outliers are listed below:

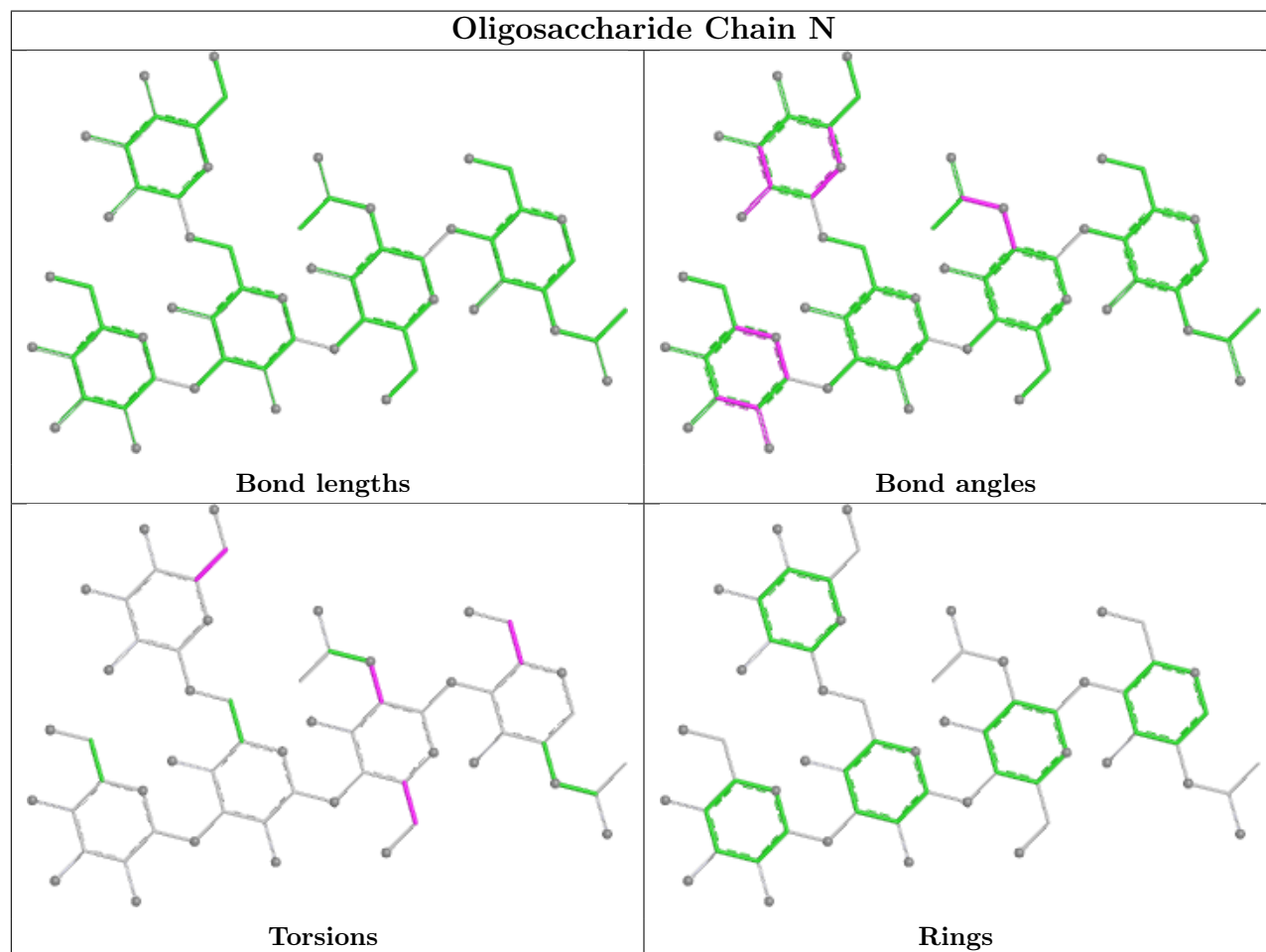
Mol	Chain	Res	Type	Atoms
6	T	1	NAG	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
5	W	3	BMA	C4-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6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

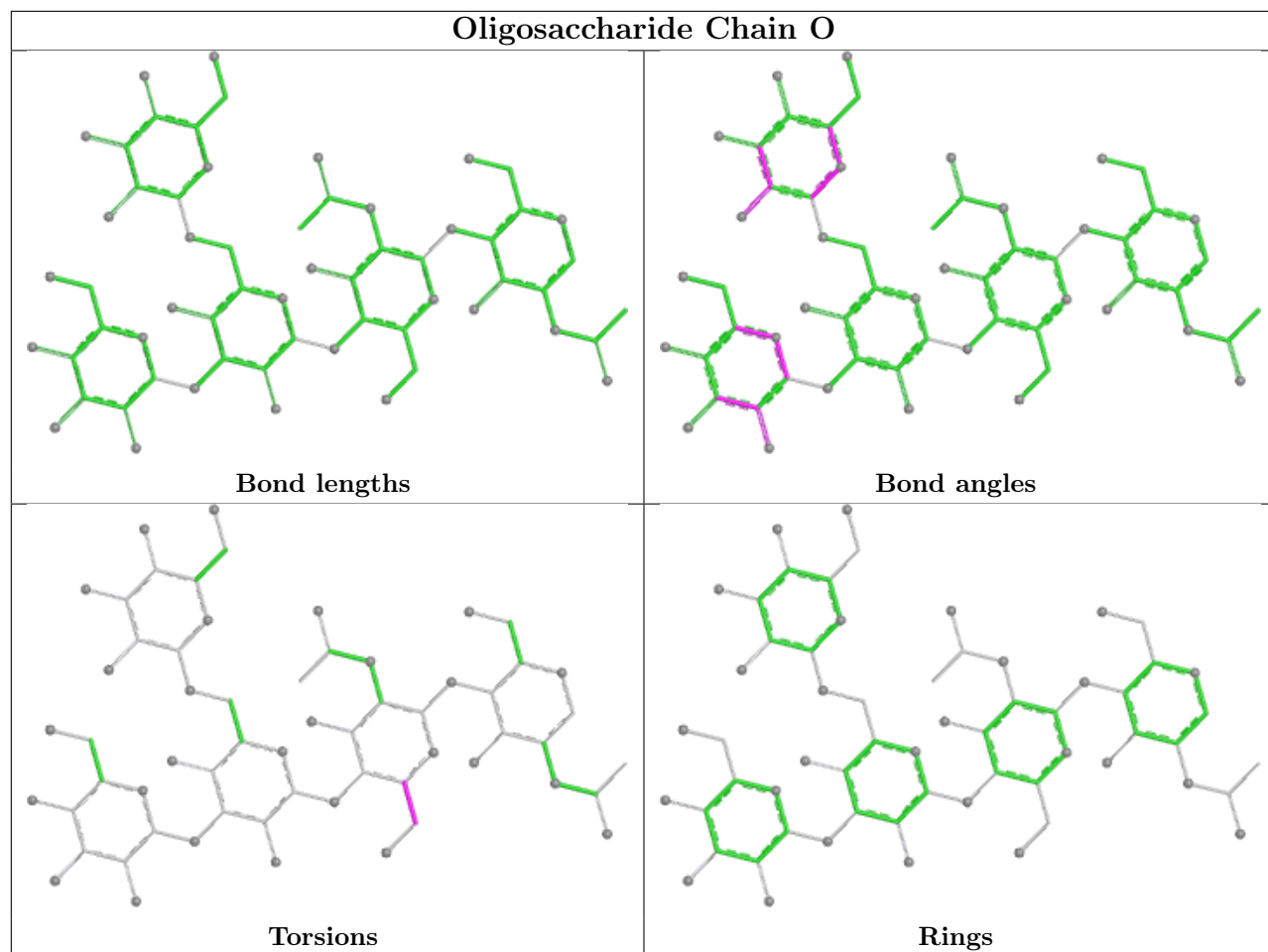
There are no ring outliers.

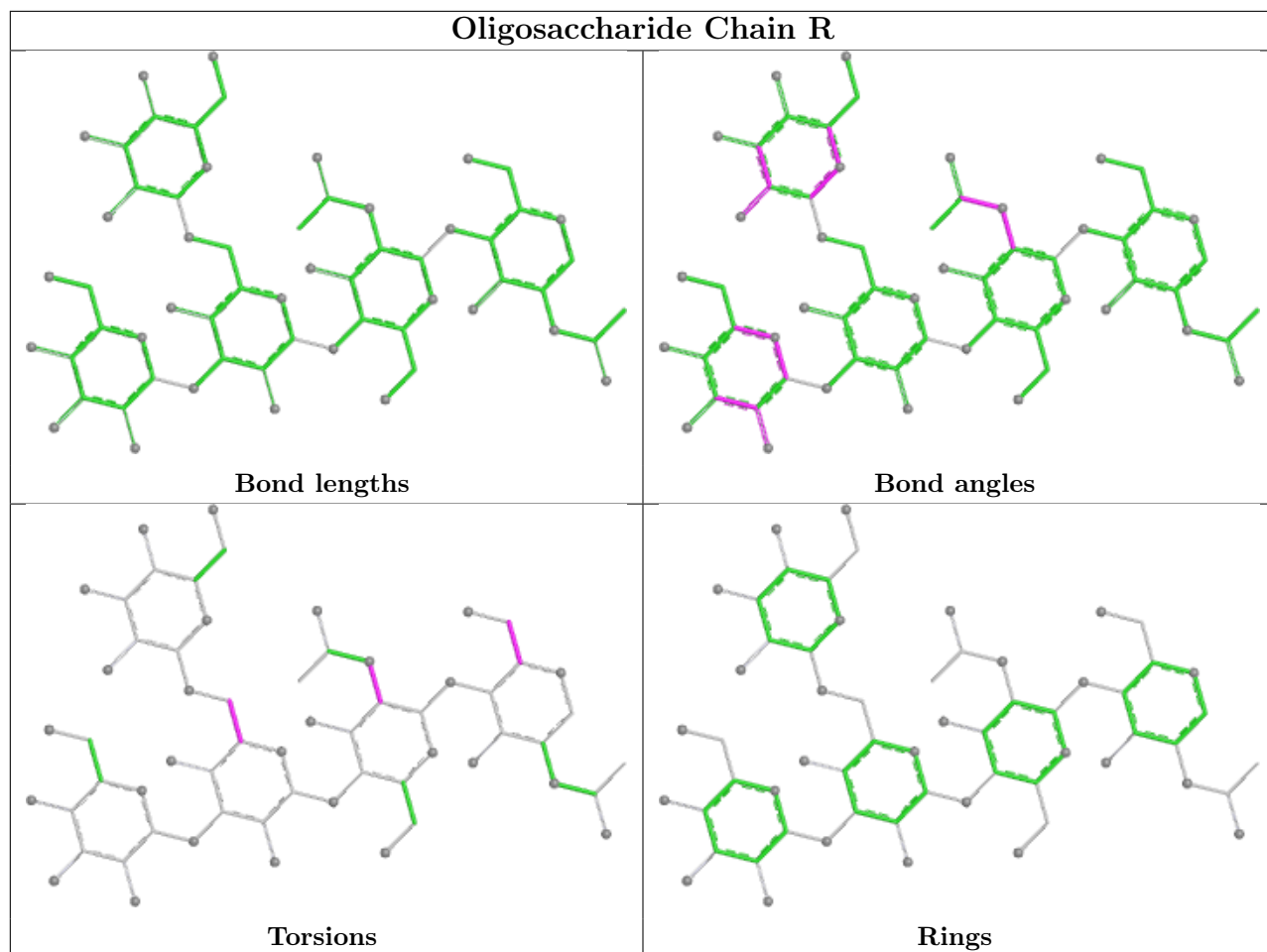
3 monomers are involved in 5 short contacts:

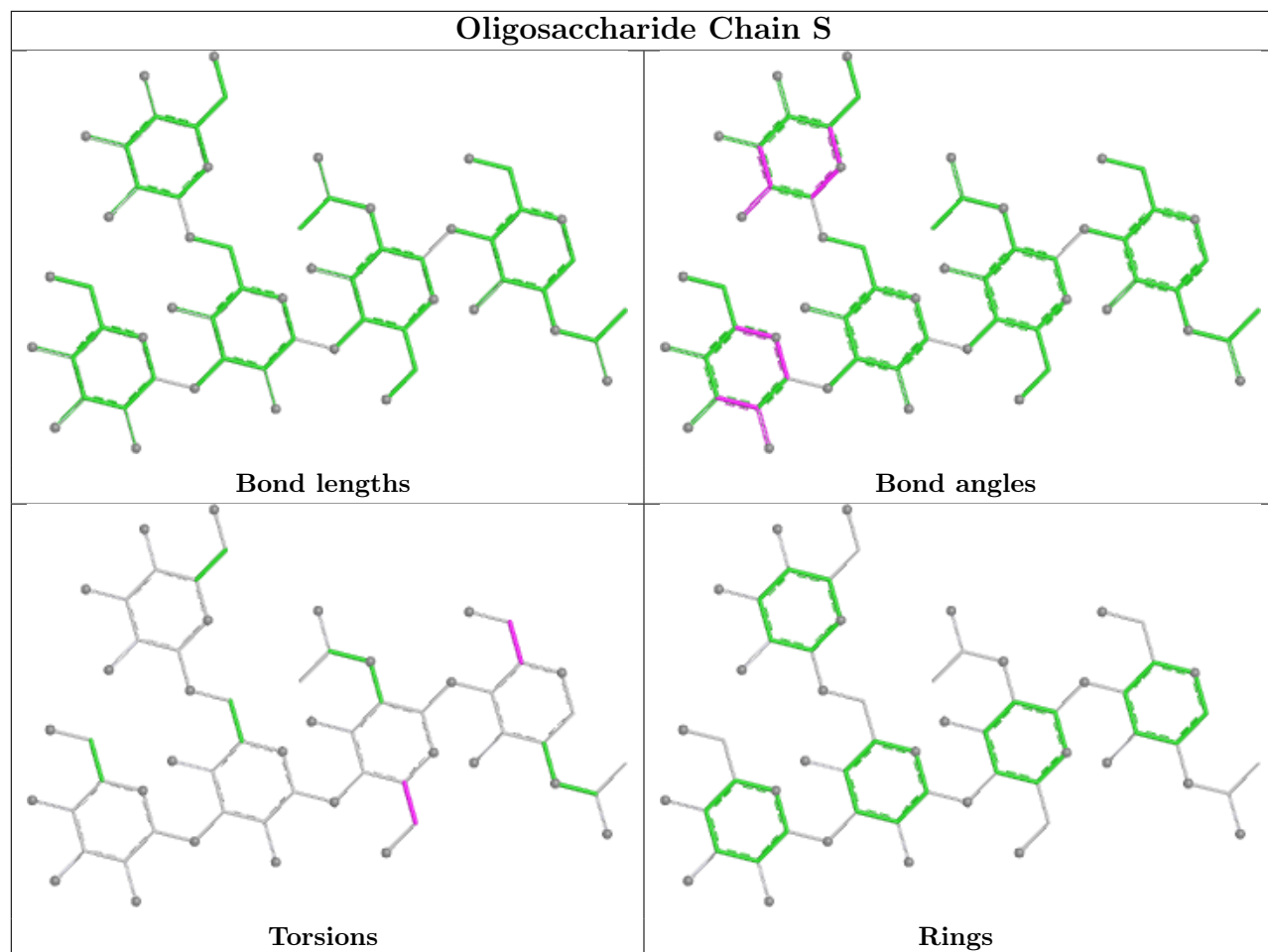
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	2	NAG	1	0
5	O	1	NAG	2	0
5	S	1	NAG	2	0

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

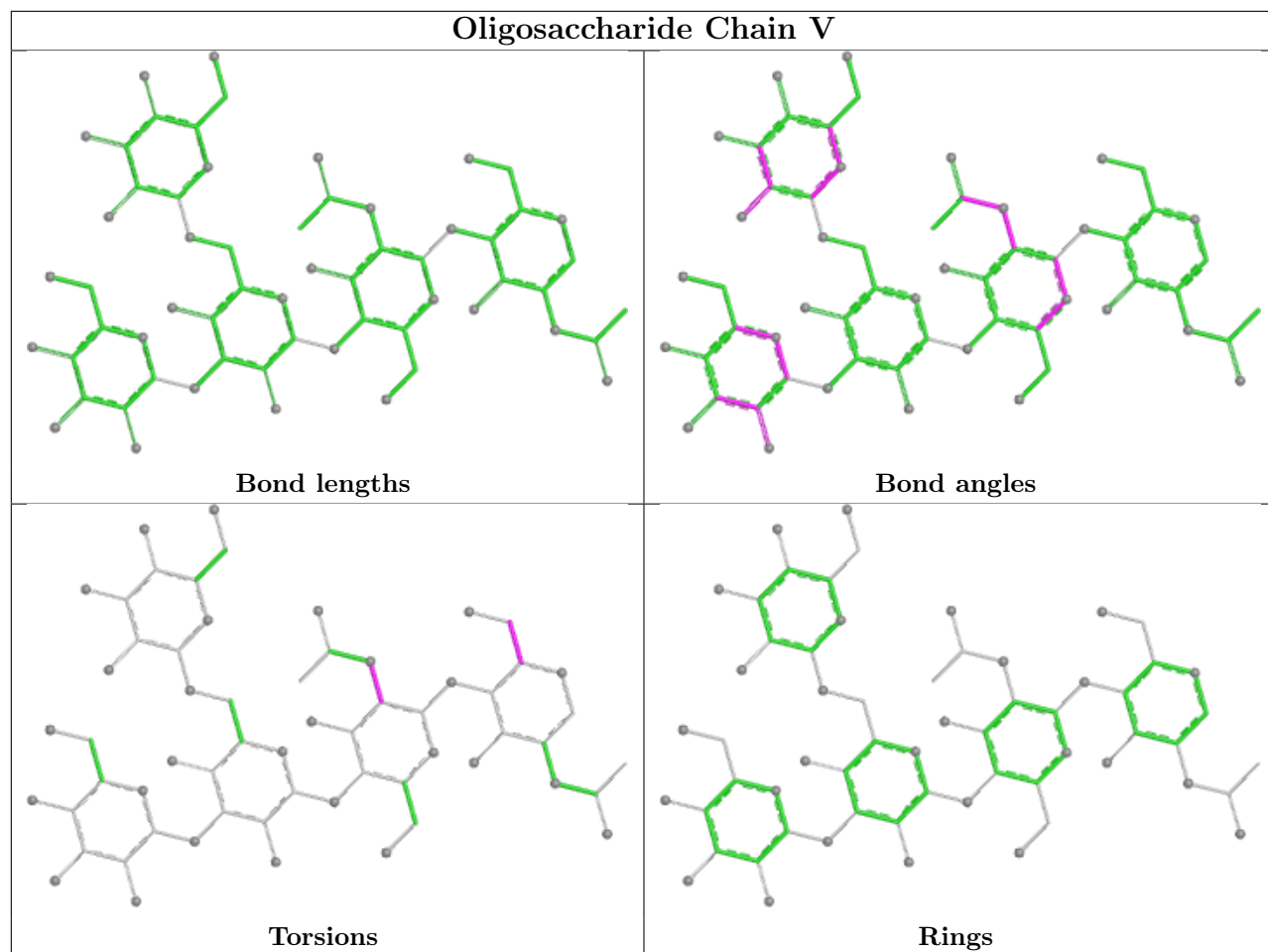


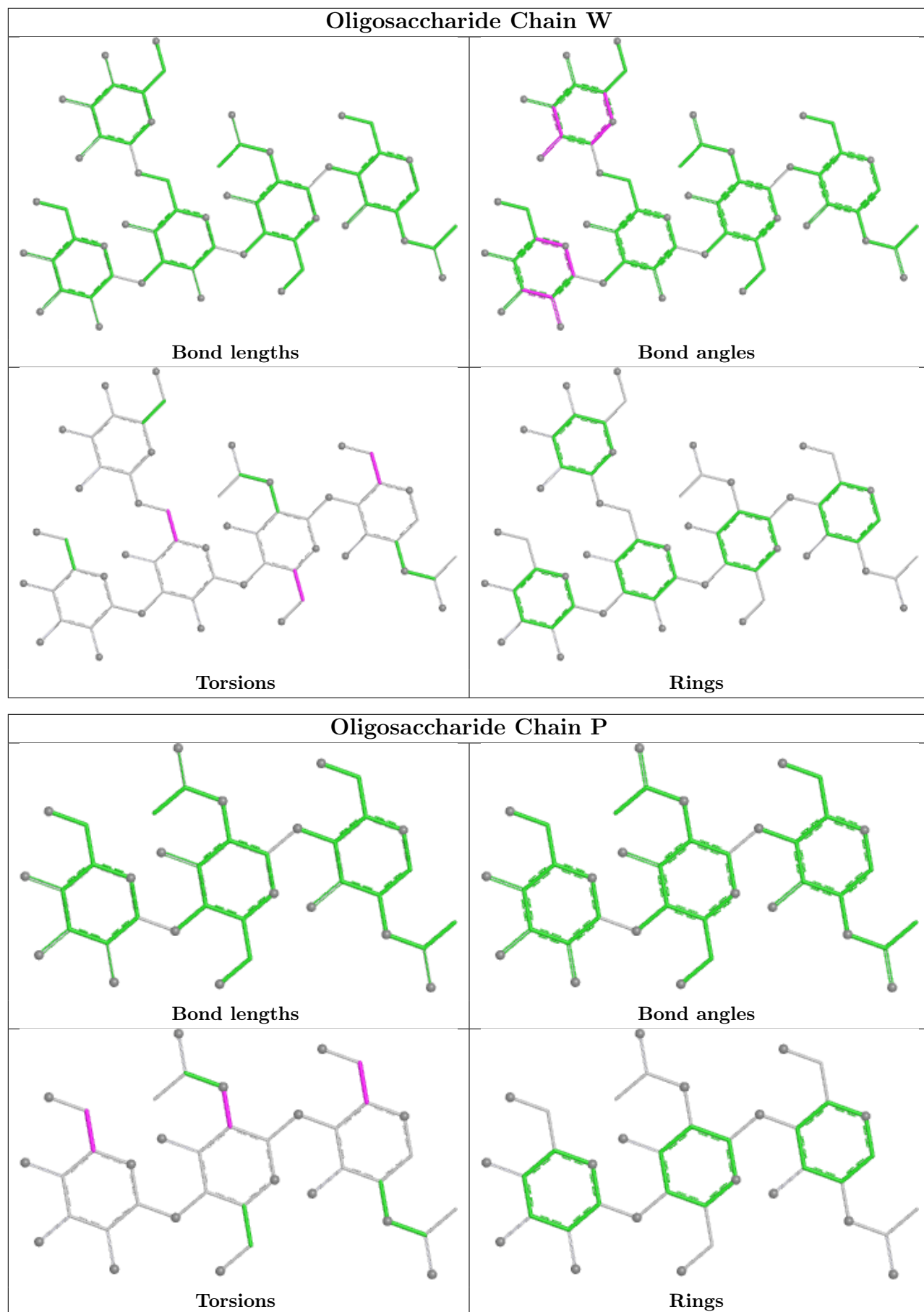


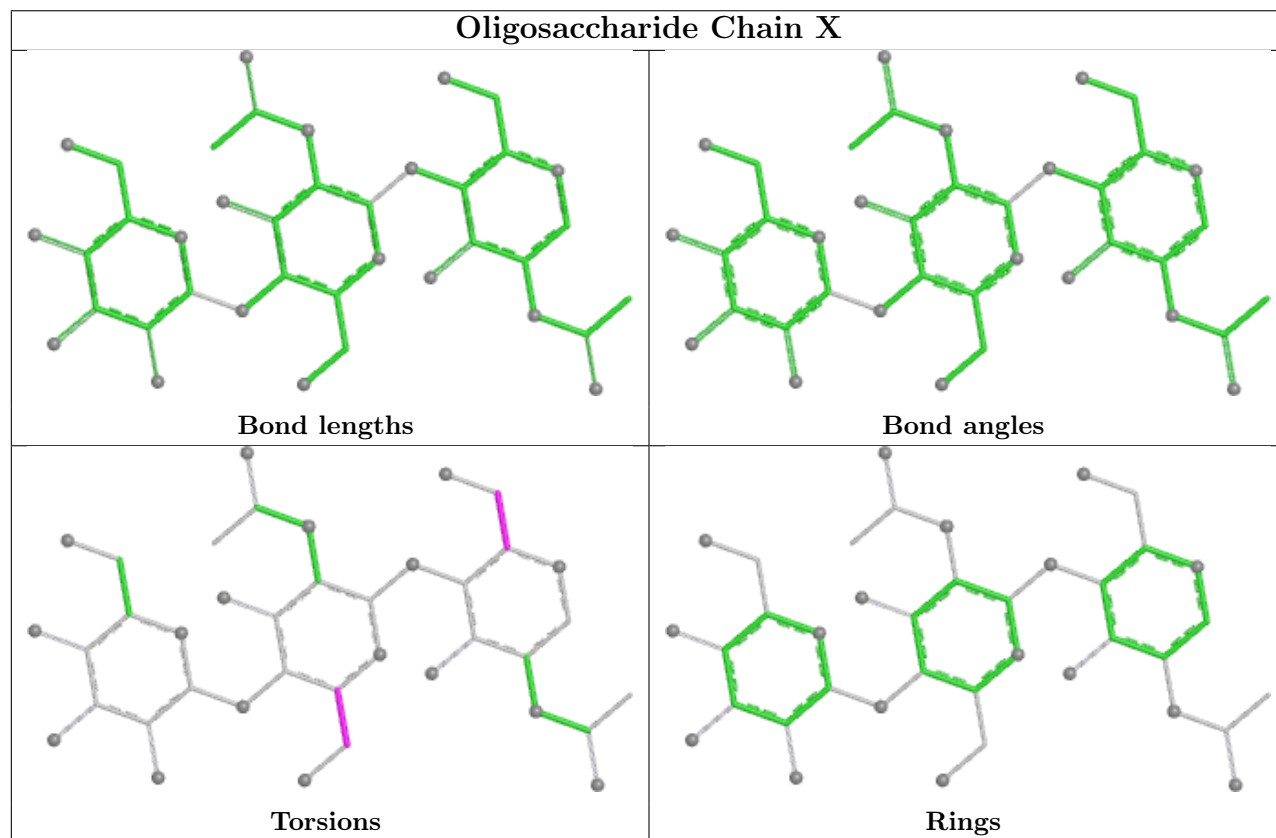
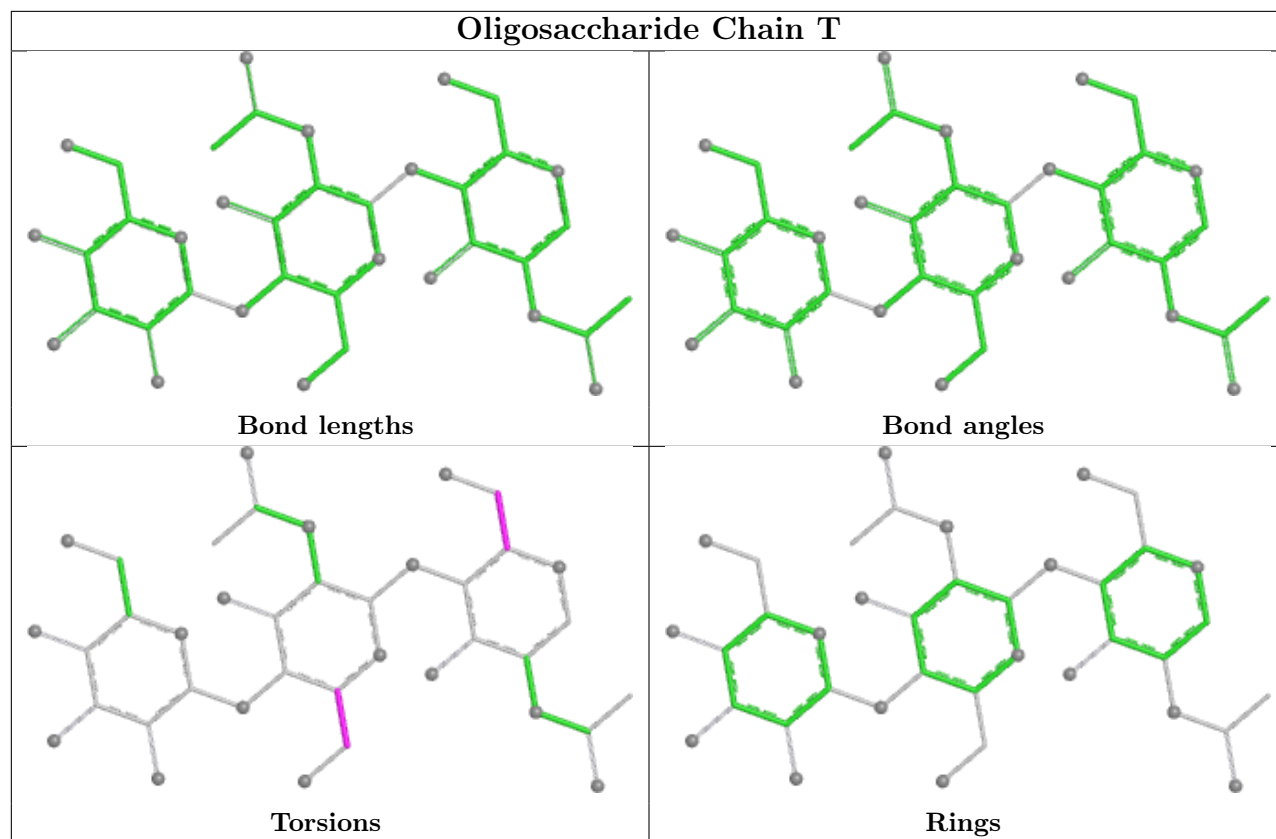












## 5.6 Ligand geometry

5 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	B	301	2	14,14,15	0.38	0	17,19,21	0.40	0
7	NAG	A	401	-	14,14,15	0.27	0	17,19,21	0.47	0
7	NAG	A	404	1	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	A	402	1	14,14,15	0.34	0	17,19,21	0.44	0
7	NAG	A	403	1	14,14,15	0.45	0	17,19,21	0.65	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	301	2	-	2/6/23/26	0/1/1/1
7	NAG	A	401	-	-	0/6/23/26	0/1/1/1
7	NAG	A	404	1	-	2/6/23/26	0/1/1/1
7	NAG	A	402	1	-	1/6/23/26	0/1/1/1
7	NAG	A	403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	403	NAG	C1-O5-C5	2.22	115.16	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	403	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	A	403	NAG	C4-C5-C6-O6
7	B	301	NAG	O5-C5-C6-O6
7	B	301	NAG	C4-C5-C6-O6
7	A	402	NAG	O5-C5-C6-O6
7	A	404	NAG	C1-C2-N2-C7
7	A	404	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

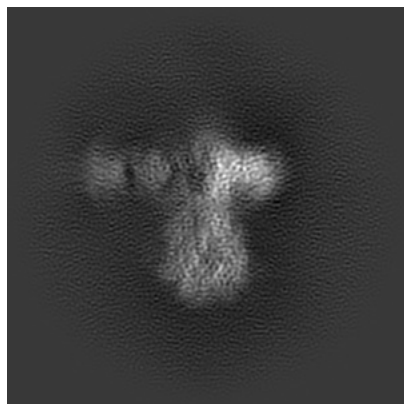
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41705. These allow visual inspection of the internal detail of the map and identification of artifacts.

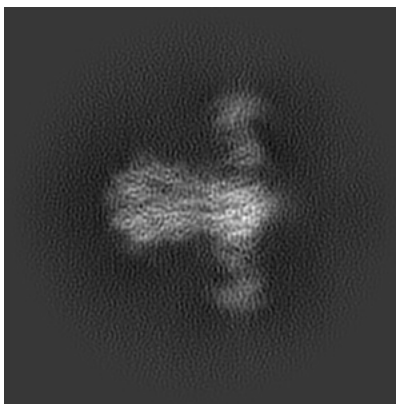
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

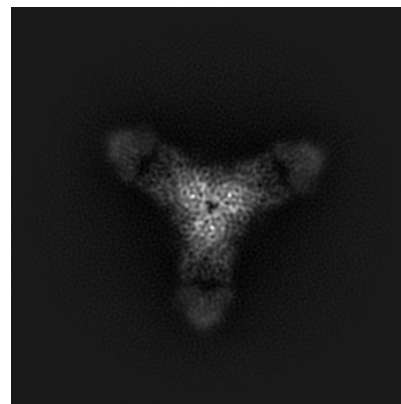
#### 6.1.1 Primary map



X

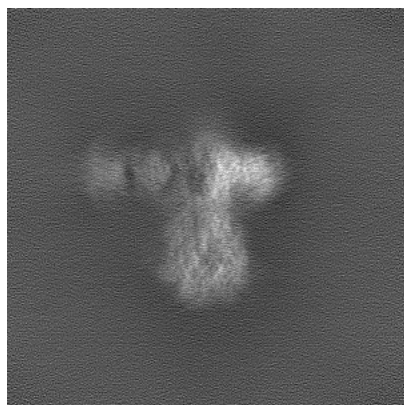


Y

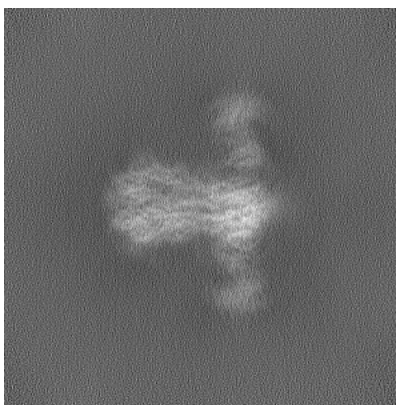


Z

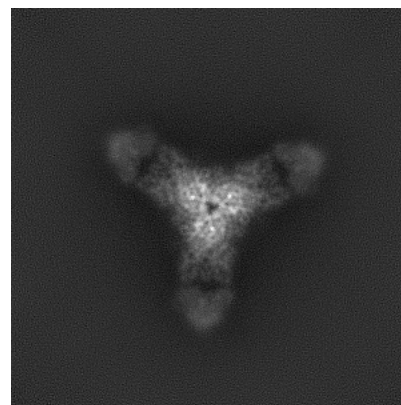
#### 6.1.2 Raw map



X



Y



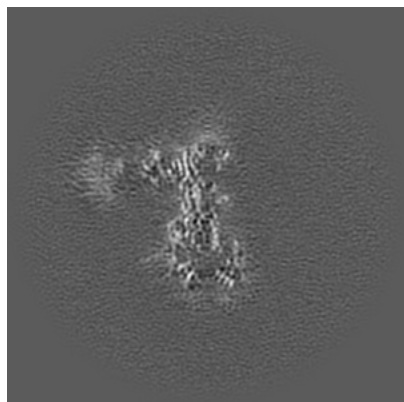
Z

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

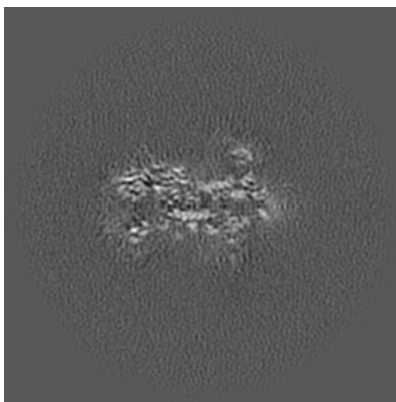


## 6.2 Central slices [i](#)

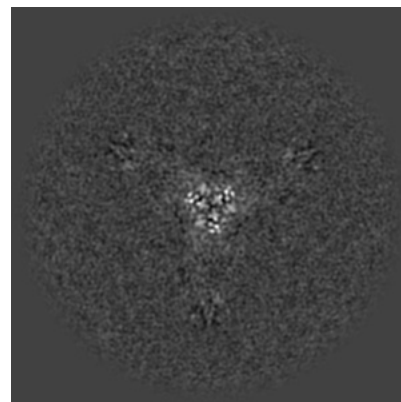
### 6.2.1 Primary map



X Index: 192

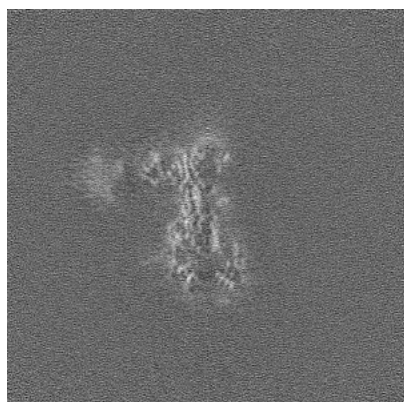


Y Index: 192

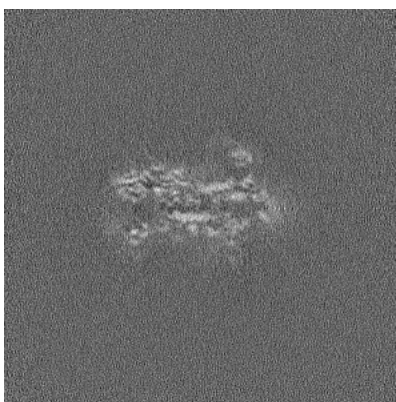


Z Index: 192

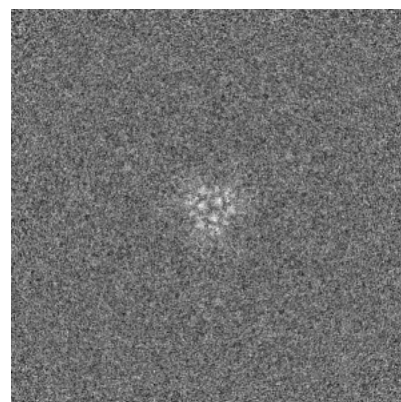
### 6.2.2 Raw map



X Index: 192



Y Index: 192

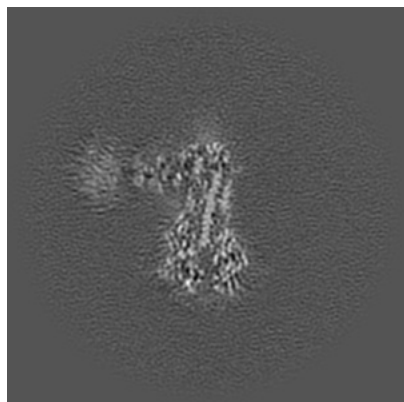


Z Index: 192

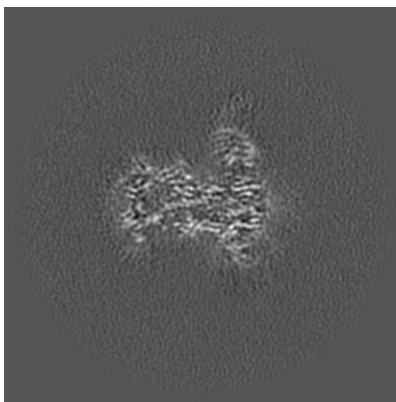
The images above show central slices of the map in three orthogonal directions.

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

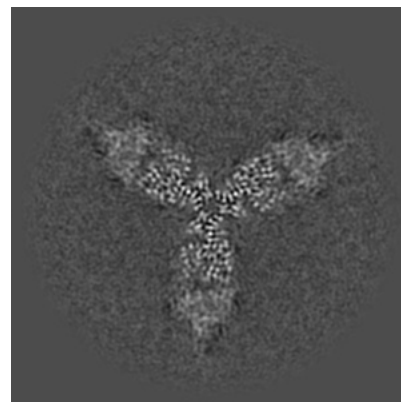
### 6.3.1 Primary map



X Index: 184

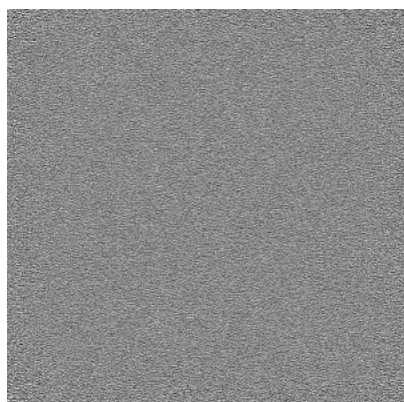


Y Index: 202

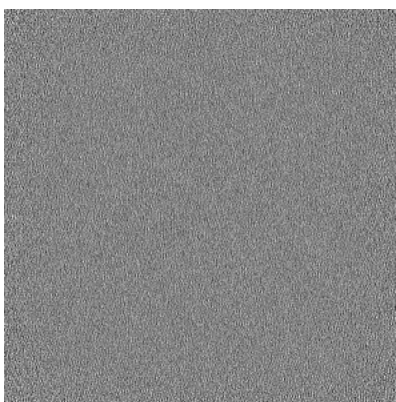


Z Index: 230

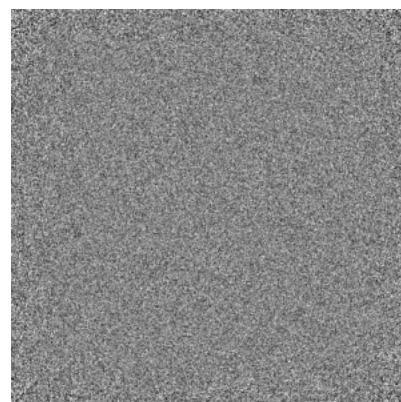
### 6.3.2 Raw map



X Index: 0



Y Index: 0



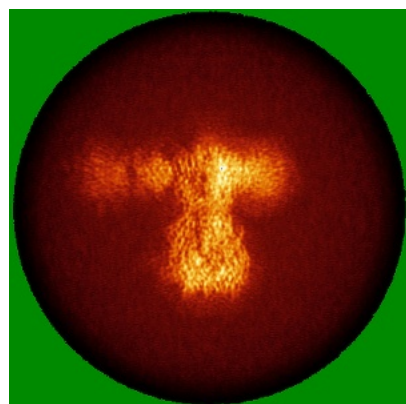
Z Index: 0

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

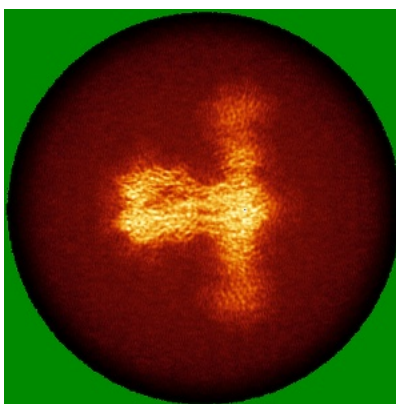


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

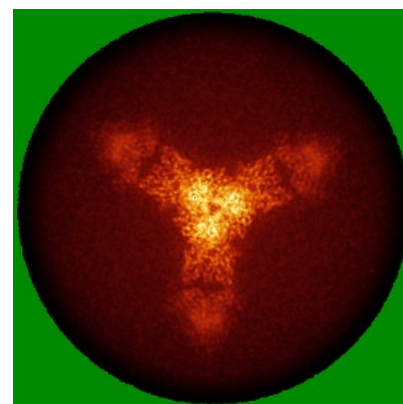
### 6.4.1 Primary map



X

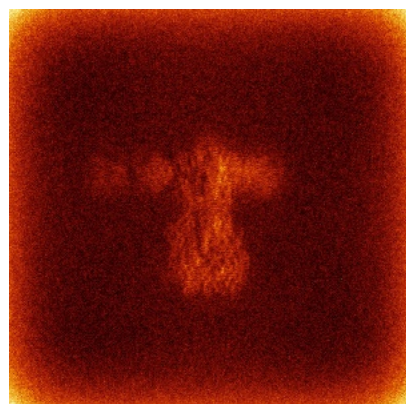


Y

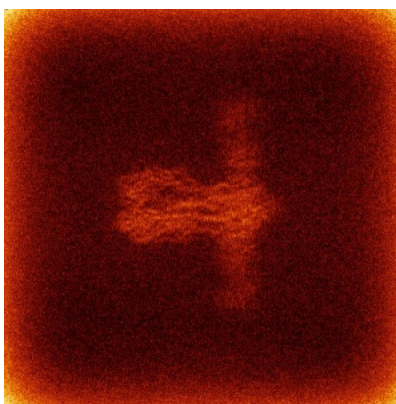


Z

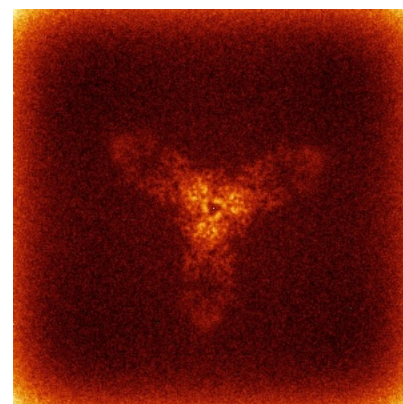
### 6.4.2 Raw map



X



Y

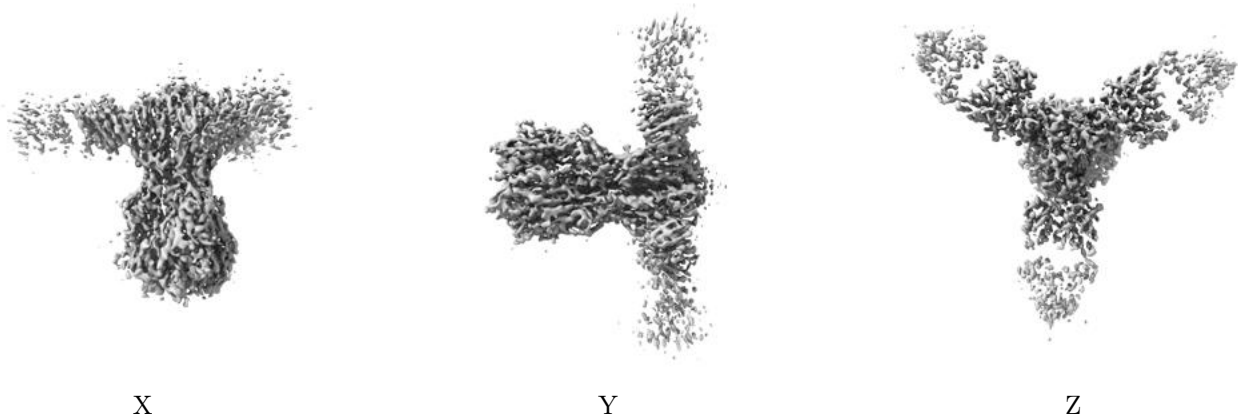


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

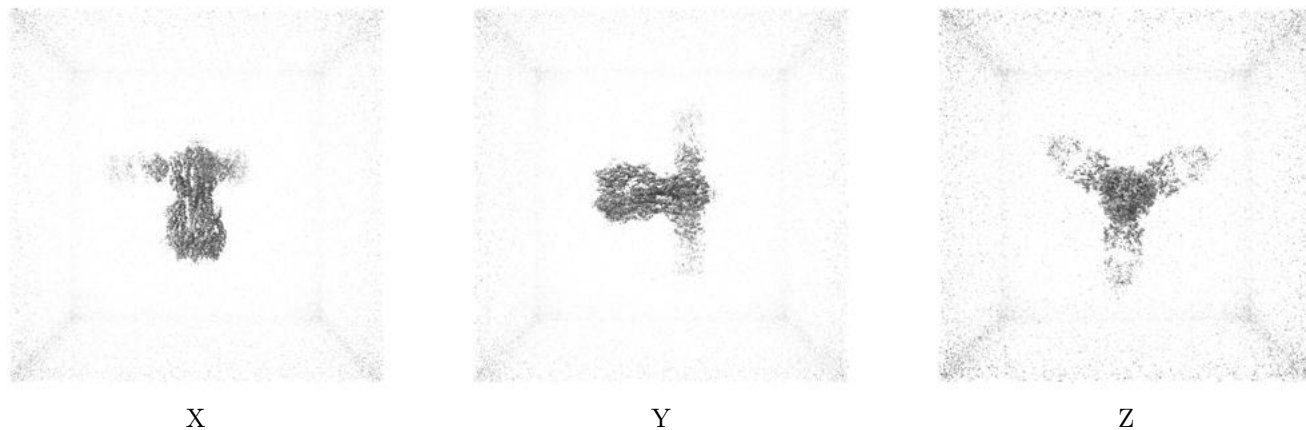
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.164. 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



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.

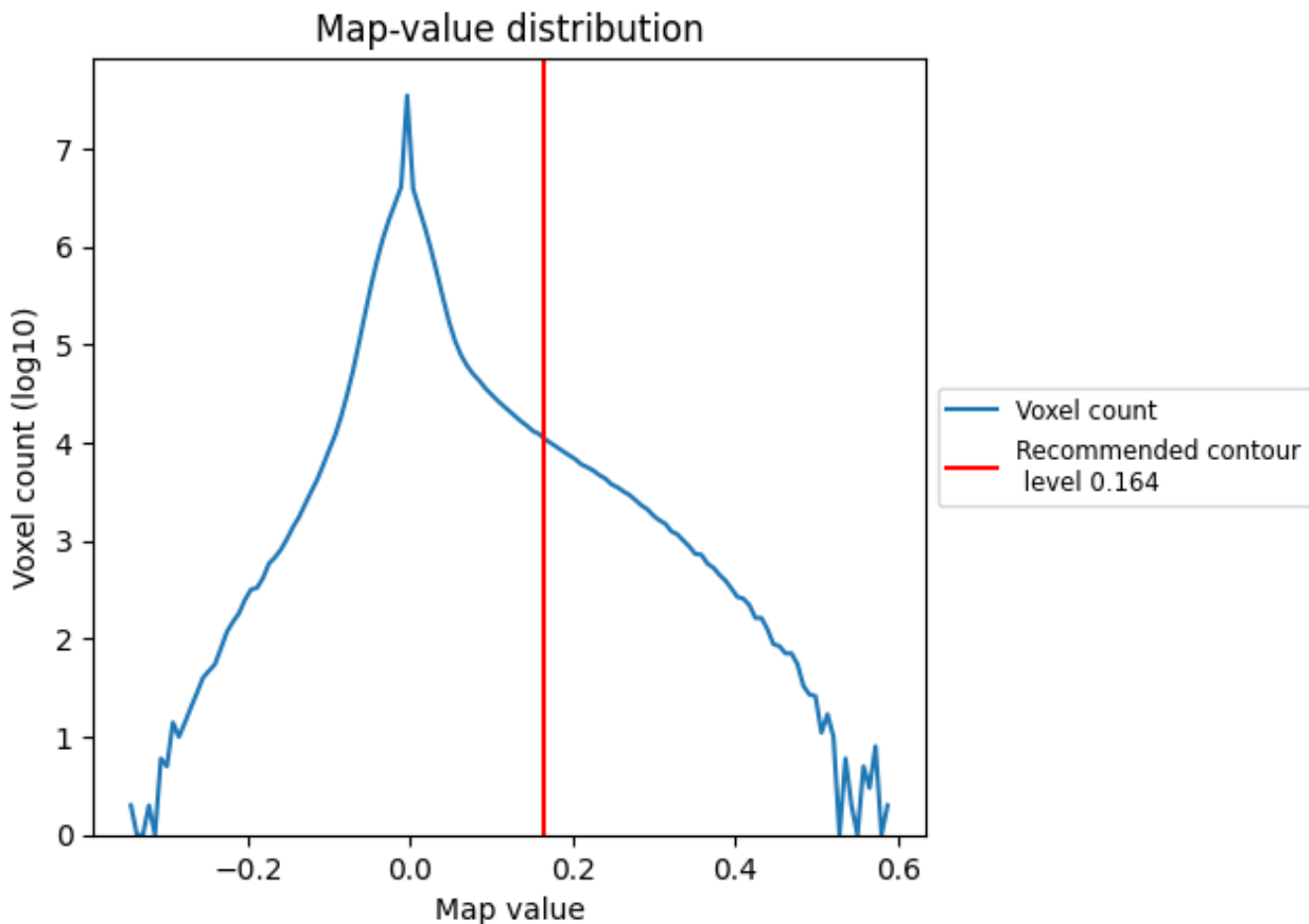
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

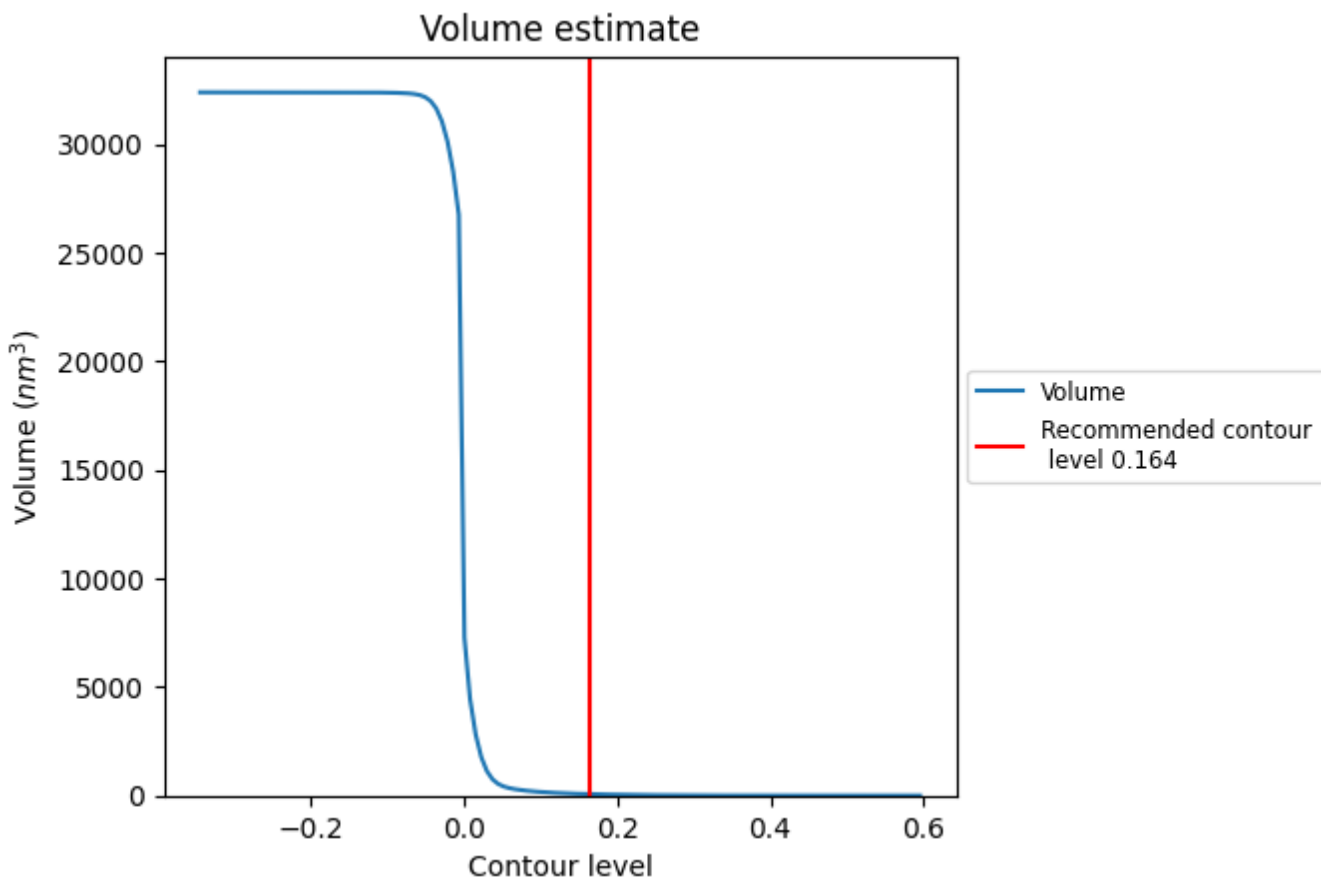
This section contains the results of statistical analysis of the map.

### 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.

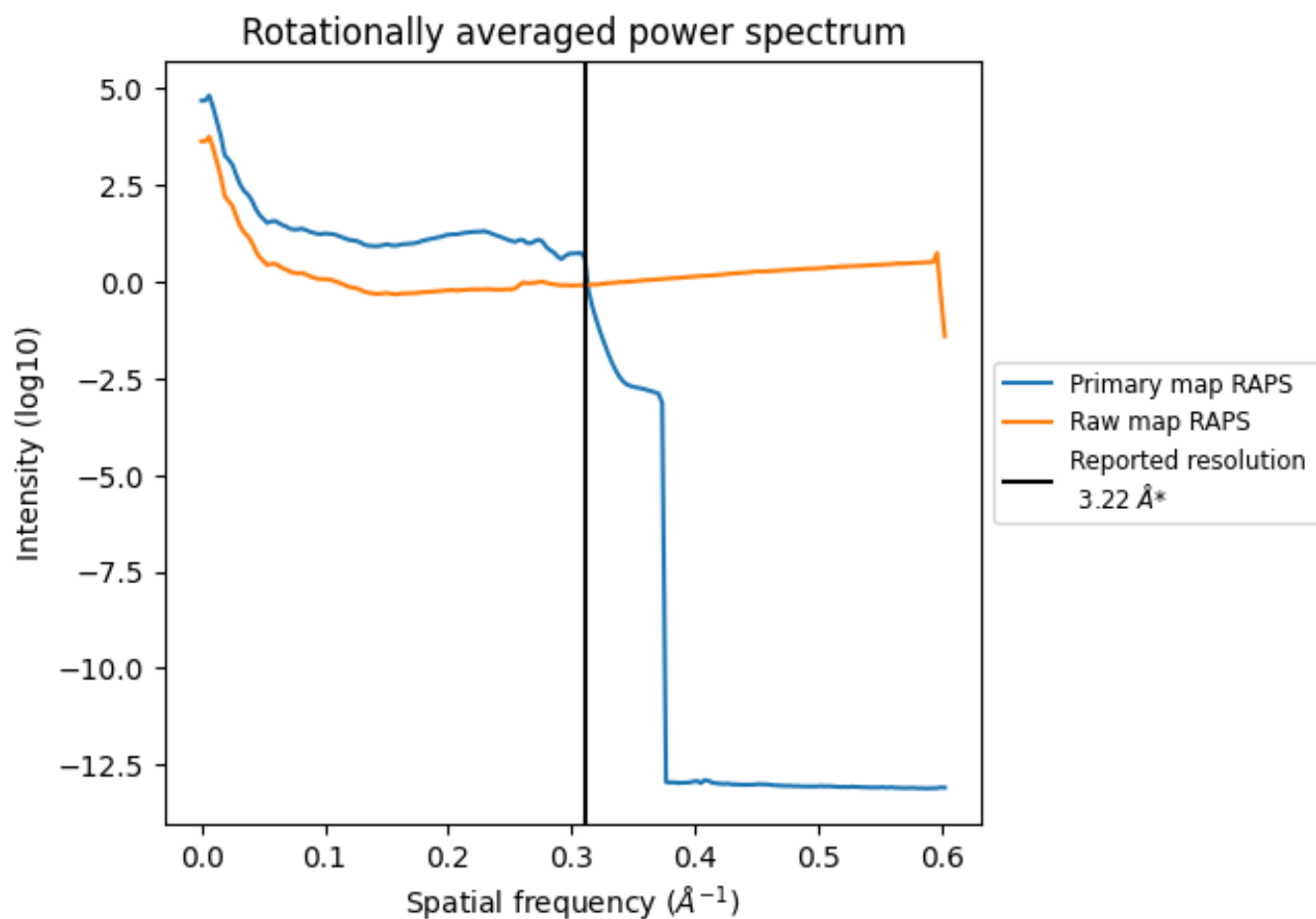
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $67 \text{ nm}^3$ ; this corresponds to an approximate mass of 60 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](#)

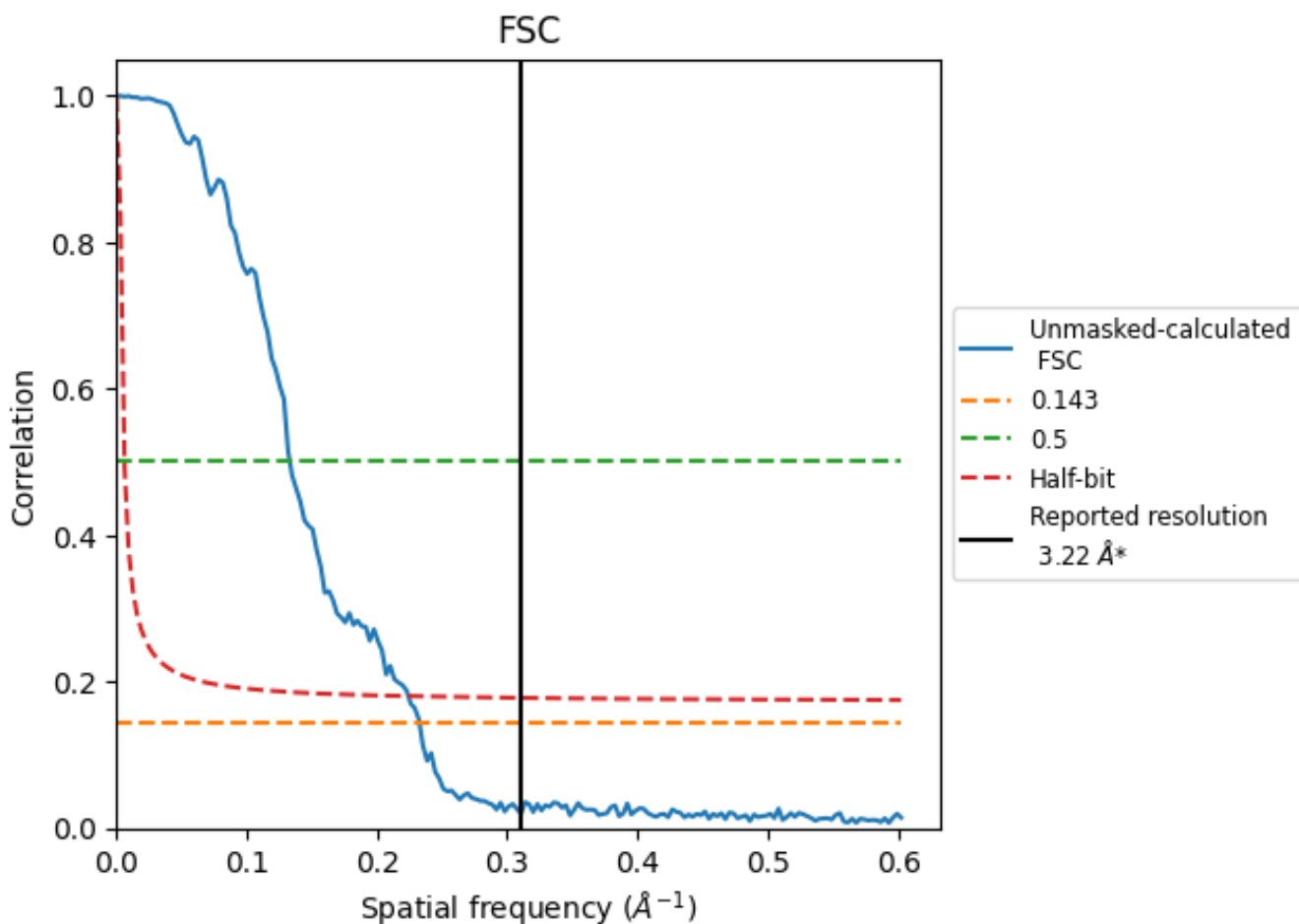


\*Reported resolution corresponds to spatial frequency of 0.311 Å<sup>-1</sup>

## 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 0.311  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

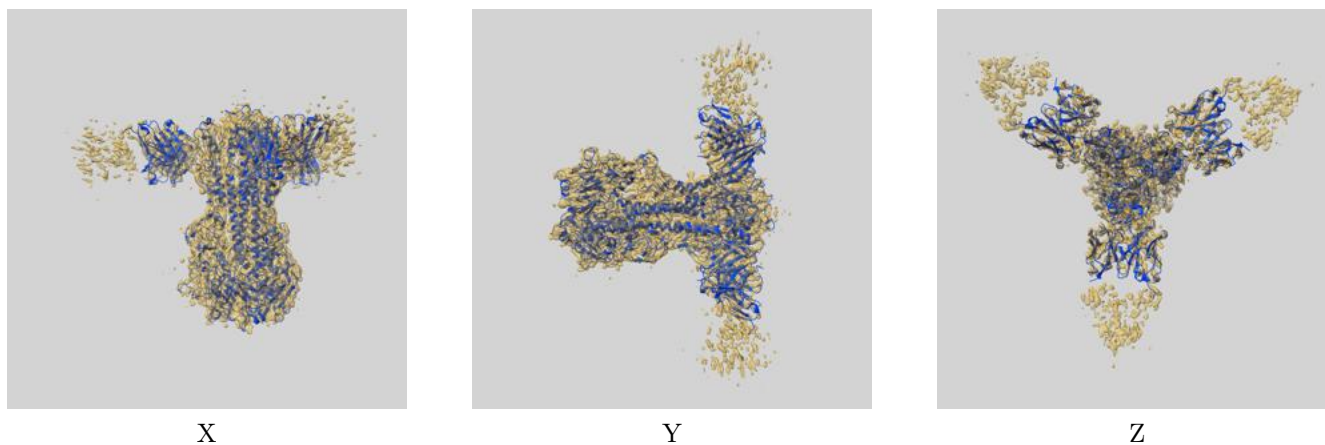
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	7.51	4.46

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.22 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-41705 and PDB model 8TXU. Per-residue inclusion information can be found in section 3 on page 12.

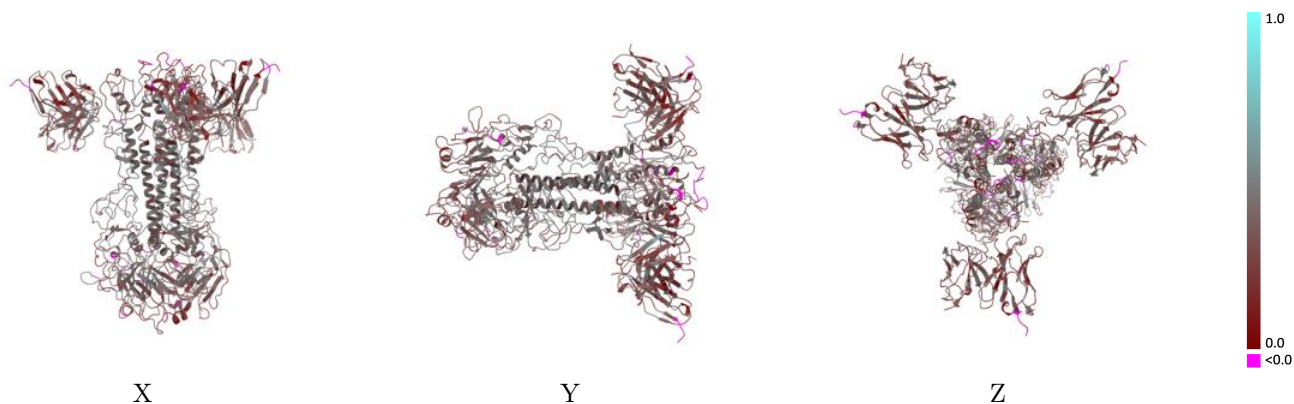
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.164 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.

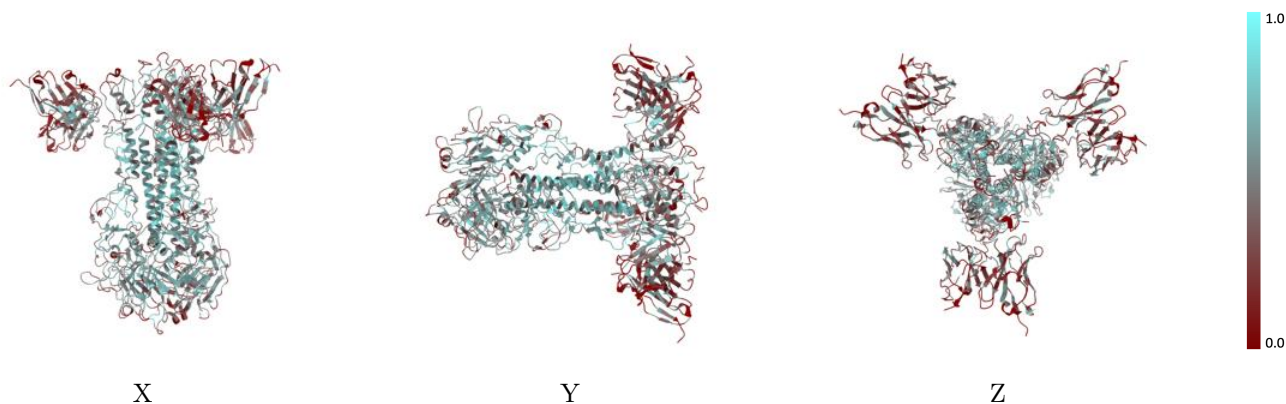


## 9.2 Q-score mapped to coordinate model [i](#)



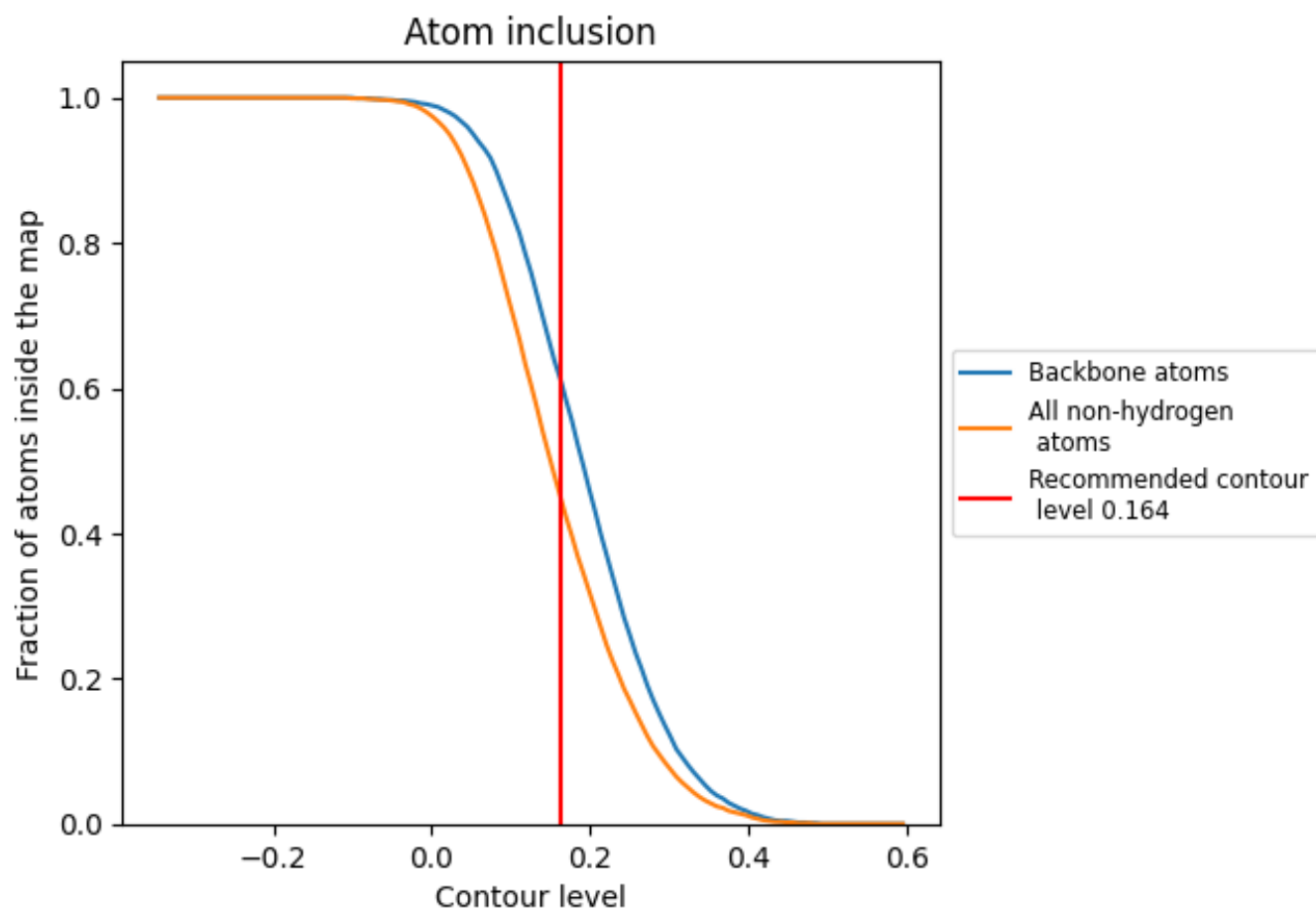
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.164).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 44% 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 (0.164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4450	 0.3480
A	 0.5170	 0.3660
B	 0.5080	 0.3590
C	 0.5210	 0.3690
D	 0.5150	 0.3590
E	 0.3510	 0.3260
F	 0.3470	 0.3150
G	 0.5170	 0.3640
H	 0.3470	 0.3210
I	 0.5110	 0.3620
J	 0.2570	 0.3060
K	 0.2710	 0.3200
L	 0.2520	 0.3110
N	 0.3280	 0.3720
O	 0.2300	 0.2440
P	 0.1540	 0.3590
R	 0.2620	 0.3250
S	 0.2300	 0.2450
T	 0.1790	 0.3530
V	 0.2790	 0.3510
W	 0.2460	 0.2360
X	 0.1540	 0.3240

