



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 12:44 PM EST

PDB ID : 7K3A
EMDB ID : EMD-22654
Title : Structure of full-length influenza HA with a head-binding antibody at pH 5.2, conformation B, fusion peptide release
Authors : Gui, M.; Gao, J.; Xiang, Y.
Deposited on : 2020-09-10
Resolution : 4.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

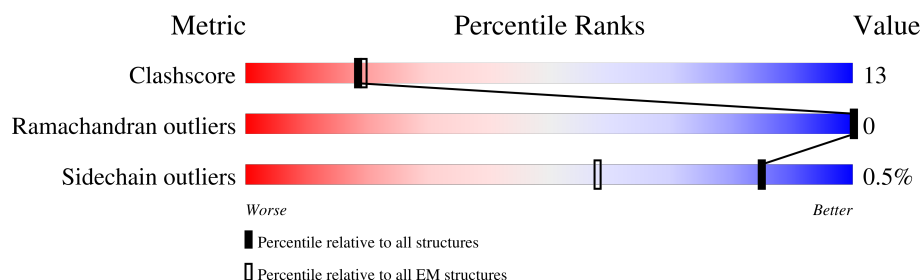
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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





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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	345	
1	C	345	
1	E	345	
2	B	254	
2	D	254	
2	F	254	
3	G	219	
3	I	219	

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Mol	Chain	Length	Quality of chain
3	K	219	
4	H	235	
4	J	235	
4	L	235	
5	M	2	
5	P	2	
5	S	2	
6	N	5	
6	Q	5	
6	T	5	
7	O	8	
7	R	8	
7	U	8	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21426 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	318	Total	C	N	O	S	0	0
			2454	1537	431	473	13		
1	C	318	Total	C	N	O	S	0	0
			2454	1537	431	473	13		
1	E	318	Total	C	N	O	S	0	0
			2454	1537	431	473	13		

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	165	Total	C	N	O	S	0	0
			1353	836	239	272	6		
2	D	165	Total	C	N	O	S	0	0
			1353	836	239	272	6		
2	F	165	Total	C	N	O	S	0	0
			1353	836	239	272	6		

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	SER	-	expression tag	UNP C7RWD9
B	223	MET	-	expression tag	UNP C7RWD9
B	224	GLY	-	expression tag	UNP C7RWD9
B	225	TRP	-	expression tag	UNP C7RWD9
B	226	SER	-	expression tag	UNP C7RWD9
B	227	HIS	-	expression tag	UNP C7RWD9
B	228	PRO	-	expression tag	UNP C7RWD9
B	229	GLN	-	expression tag	UNP C7RWD9
B	230	PHE	-	expression tag	UNP C7RWD9
B	231	GLU	-	expression tag	UNP C7RWD9
B	232	LYS	-	expression tag	UNP C7RWD9
B	233	GLY	-	expression tag	UNP C7RWD9
B	234	GLY	-	expression tag	UNP C7RWD9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	235	GLY	-	expression tag	UNP C7RWD9
B	236	ALA	-	expression tag	UNP C7RWD9
B	237	ARG	-	expression tag	UNP C7RWD9
B	238	GLY	-	expression tag	UNP C7RWD9
B	239	GLY	-	expression tag	UNP C7RWD9
B	240	SER	-	expression tag	UNP C7RWD9
B	241	GLY	-	expression tag	UNP C7RWD9
B	242	GLY	-	expression tag	UNP C7RWD9
B	243	GLY	-	expression tag	UNP C7RWD9
B	244	SER	-	expression tag	UNP C7RWD9
B	245	TRP	-	expression tag	UNP C7RWD9
B	246	SER	-	expression tag	UNP C7RWD9
B	247	HIS	-	expression tag	UNP C7RWD9
B	248	PRO	-	expression tag	UNP C7RWD9
B	249	GLN	-	expression tag	UNP C7RWD9
B	250	PHE	-	expression tag	UNP C7RWD9
B	251	GLU	-	expression tag	UNP C7RWD9
B	252	LYS	-	expression tag	UNP C7RWD9
B	253	GLY	-	expression tag	UNP C7RWD9
B	254	PHE	-	expression tag	UNP C7RWD9
D	222	SER	-	expression tag	UNP C7RWD9
D	223	MET	-	expression tag	UNP C7RWD9
D	224	GLY	-	expression tag	UNP C7RWD9
D	225	TRP	-	expression tag	UNP C7RWD9
D	226	SER	-	expression tag	UNP C7RWD9
D	227	HIS	-	expression tag	UNP C7RWD9
D	228	PRO	-	expression tag	UNP C7RWD9
D	229	GLN	-	expression tag	UNP C7RWD9
D	230	PHE	-	expression tag	UNP C7RWD9
D	231	GLU	-	expression tag	UNP C7RWD9
D	232	LYS	-	expression tag	UNP C7RWD9
D	233	GLY	-	expression tag	UNP C7RWD9
D	234	GLY	-	expression tag	UNP C7RWD9
D	235	GLY	-	expression tag	UNP C7RWD9
D	236	ALA	-	expression tag	UNP C7RWD9
D	237	ARG	-	expression tag	UNP C7RWD9
D	238	GLY	-	expression tag	UNP C7RWD9
D	239	GLY	-	expression tag	UNP C7RWD9
D	240	SER	-	expression tag	UNP C7RWD9
D	241	GLY	-	expression tag	UNP C7RWD9
D	242	GLY	-	expression tag	UNP C7RWD9
D	243	GLY	-	expression tag	UNP C7RWD9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	244	SER	-	expression tag	UNP C7RWD9
D	245	TRP	-	expression tag	UNP C7RWD9
D	246	SER	-	expression tag	UNP C7RWD9
D	247	HIS	-	expression tag	UNP C7RWD9
D	248	PRO	-	expression tag	UNP C7RWD9
D	249	GLN	-	expression tag	UNP C7RWD9
D	250	PHE	-	expression tag	UNP C7RWD9
D	251	GLU	-	expression tag	UNP C7RWD9
D	252	LYS	-	expression tag	UNP C7RWD9
D	253	GLY	-	expression tag	UNP C7RWD9
D	254	PHE	-	expression tag	UNP C7RWD9
F	222	SER	-	expression tag	UNP C7RWD9
F	223	MET	-	expression tag	UNP C7RWD9
F	224	GLY	-	expression tag	UNP C7RWD9
F	225	TRP	-	expression tag	UNP C7RWD9
F	226	SER	-	expression tag	UNP C7RWD9
F	227	HIS	-	expression tag	UNP C7RWD9
F	228	PRO	-	expression tag	UNP C7RWD9
F	229	GLN	-	expression tag	UNP C7RWD9
F	230	PHE	-	expression tag	UNP C7RWD9
F	231	GLU	-	expression tag	UNP C7RWD9
F	232	LYS	-	expression tag	UNP C7RWD9
F	233	GLY	-	expression tag	UNP C7RWD9
F	234	GLY	-	expression tag	UNP C7RWD9
F	235	GLY	-	expression tag	UNP C7RWD9
F	236	ALA	-	expression tag	UNP C7RWD9
F	237	ARG	-	expression tag	UNP C7RWD9
F	238	GLY	-	expression tag	UNP C7RWD9
F	239	GLY	-	expression tag	UNP C7RWD9
F	240	SER	-	expression tag	UNP C7RWD9
F	241	GLY	-	expression tag	UNP C7RWD9
F	242	GLY	-	expression tag	UNP C7RWD9
F	243	GLY	-	expression tag	UNP C7RWD9
F	244	SER	-	expression tag	UNP C7RWD9
F	245	TRP	-	expression tag	UNP C7RWD9
F	246	SER	-	expression tag	UNP C7RWD9
F	247	HIS	-	expression tag	UNP C7RWD9
F	248	PRO	-	expression tag	UNP C7RWD9
F	249	GLN	-	expression tag	UNP C7RWD9
F	250	PHE	-	expression tag	UNP C7RWD9
F	251	GLU	-	expression tag	UNP C7RWD9
F	252	LYS	-	expression tag	UNP C7RWD9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	253	GLY	-	expression tag	UNP C7RWD9
F	254	PHE	-	expression tag	UNP C7RWD9

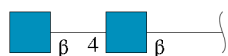
- Molecule 3 is a protein called antibody Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	202	Total	C	N	O	S	2	0
			1502	932	258	308	4		
3	I	202	Total	C	N	O	S	2	0
			1502	932	258	308	4		
3	K	202	Total	C	N	O	S	2	0
			1502	932	258	308	4		

- Molecule 4 is a protein called antibody Fab heavy chain.

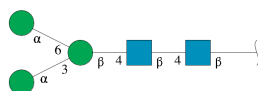
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	212	Total	C	N	O	S	0	0
			1608	1022	269	307	10		
4	J	212	Total	C	N	O	S	0	0
			1608	1022	269	307	10		
4	L	212	Total	C	N	O	S	0	0
			1608	1022	269	307	10		

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



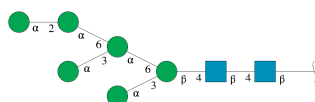
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		

- 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
6	N	5	Total	C	N	O	0	0
			61	34	2	25		
6	Q	5	Total	C	N	O	0	0
			61	34	2	25		
6	T	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	8	Total	C	N	O	0	0
			94	52	2	40		
7	R	8	Total	C	N	O	0	0
			94	52	2	40		
7	U	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

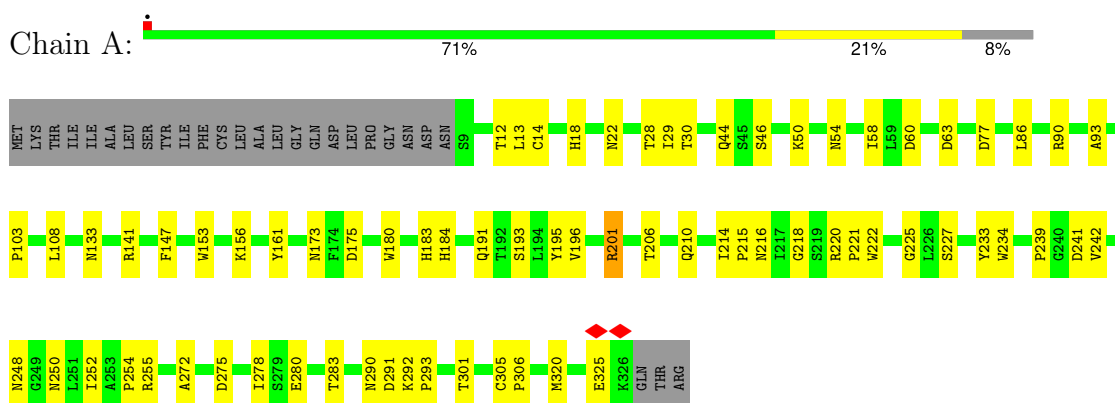


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8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

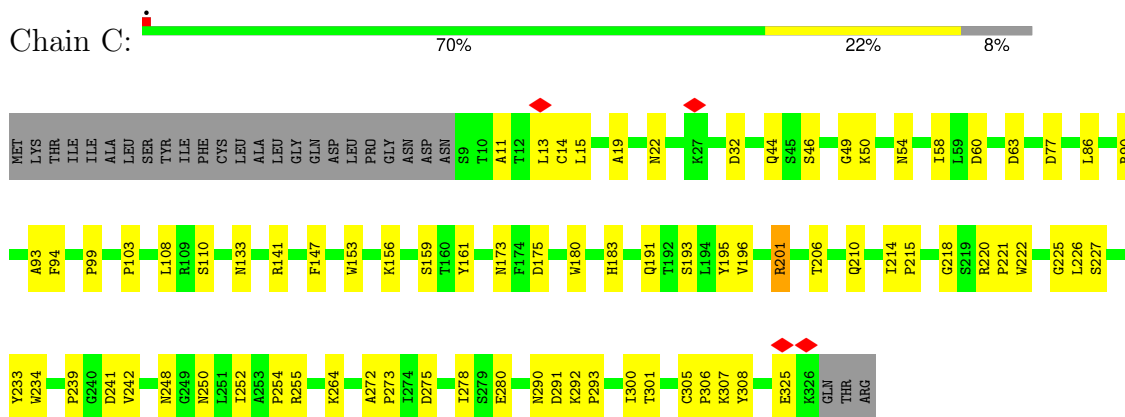
3 Residue-property plots

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.

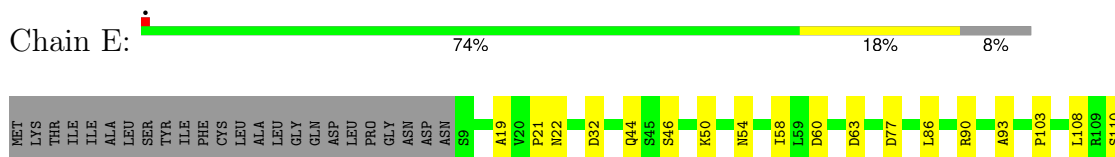
• Molecule 1: Hemagglutinin

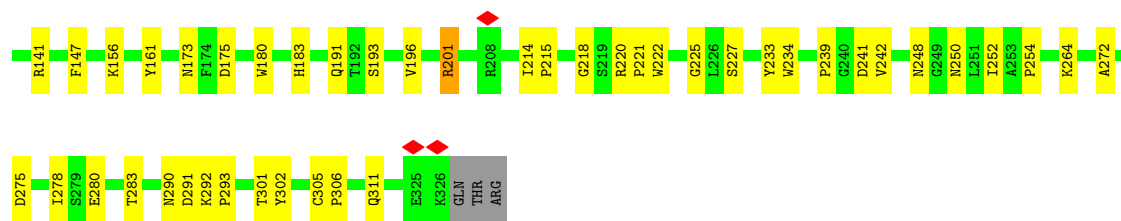


• Molecule 1: Hemagglutinin

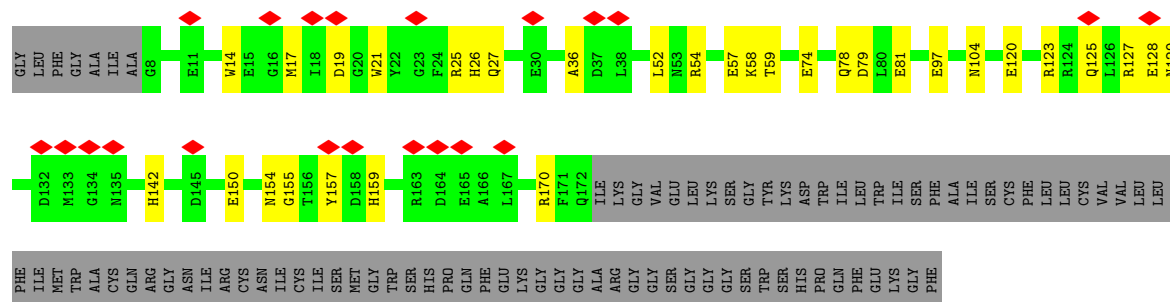


• Molecule 1: Hemagglutinin

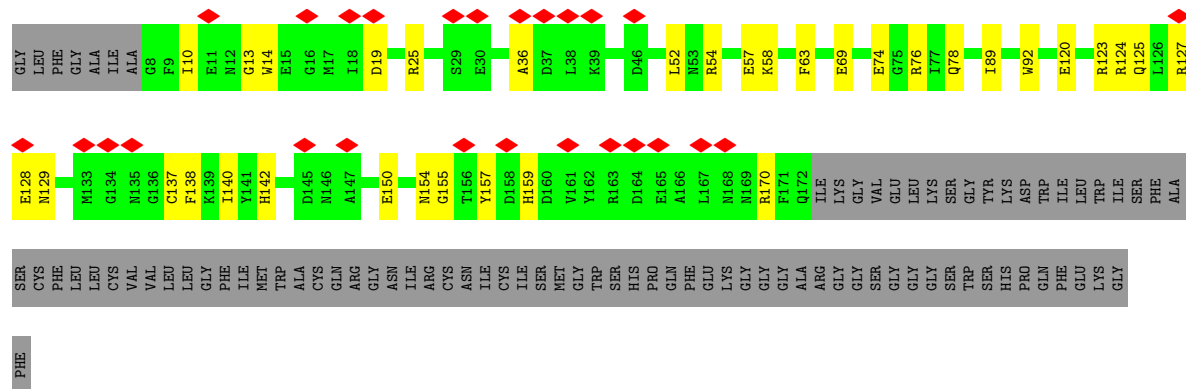




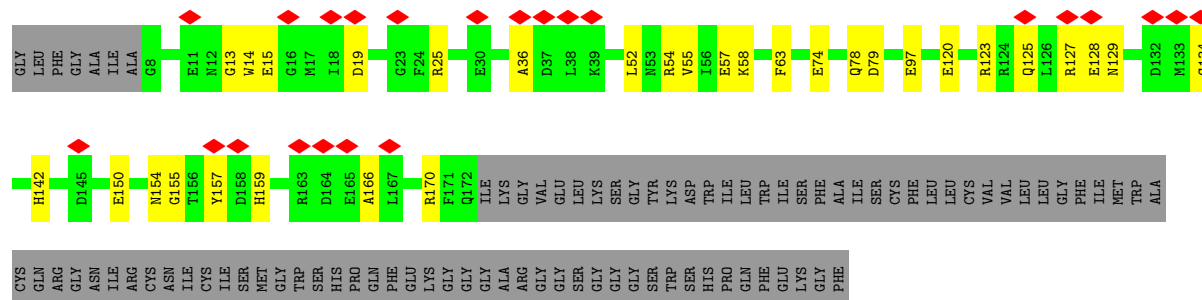
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



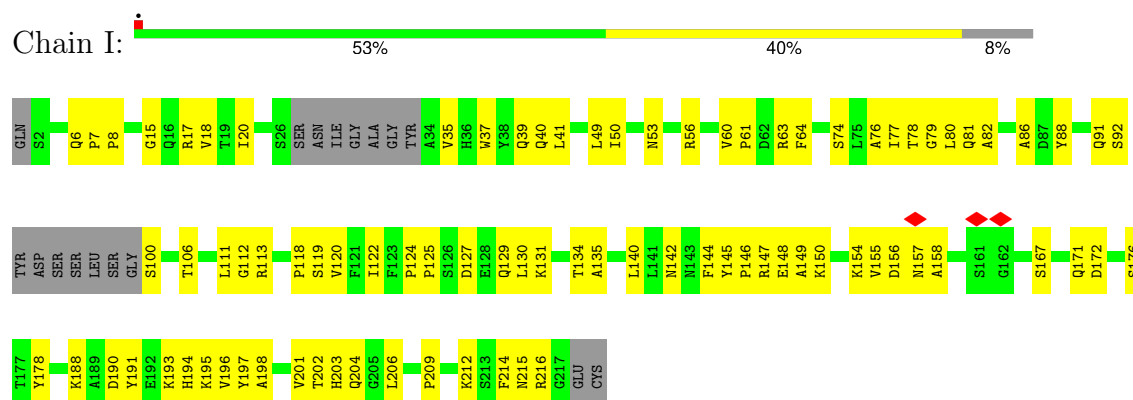
• Molecule 2: Hemagglutinin



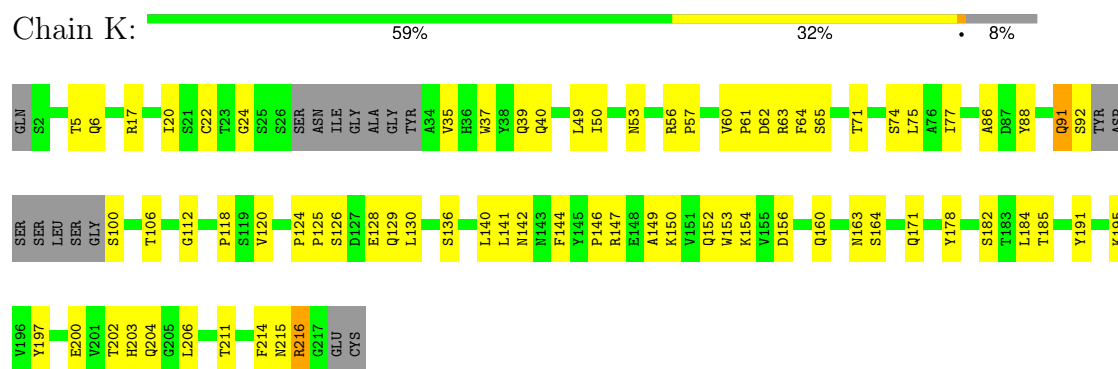
- Molecule 3: antibody Fab light chain



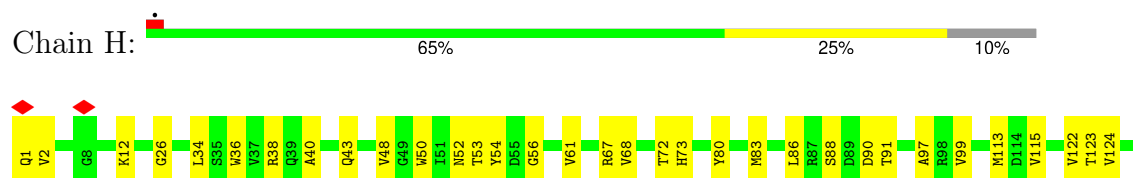
- Molecule 3: antibody Fab light chain

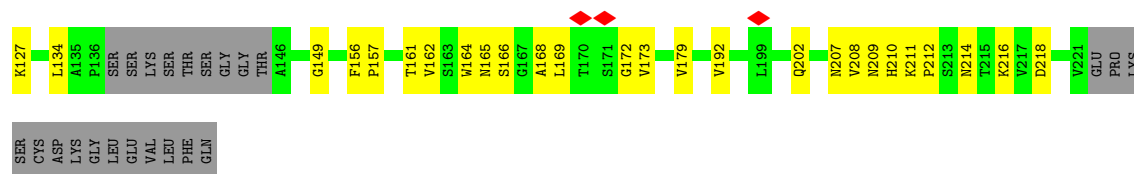


- Molecule 3: antibody Fab light chain

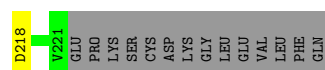
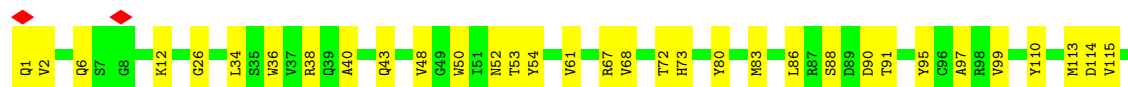


- Molecule 4: antibody Fab heavy chain

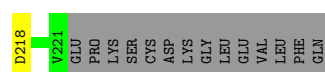
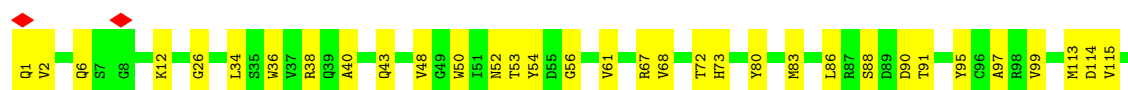




• Molecule 4: antibody Fab heavy chain



• Molecule 4: antibody Fab heavy chain



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



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





- 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



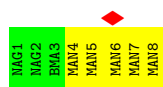
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



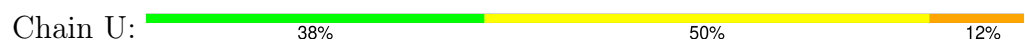
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	14650	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	399.0, 399.0, 399.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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	0.28	0/2510	0.49	0/3420
1	C	0.28	0/2510	0.49	0/3420
1	E	0.28	0/2510	0.49	0/3420
2	B	0.27	0/1376	0.44	0/1849
2	D	0.27	0/1376	0.44	0/1849
2	F	0.27	0/1376	0.44	0/1849
3	G	0.29	0/1531	0.52	0/2079
3	I	0.29	0/1531	0.54	0/2079
3	K	0.28	0/1531	0.52	0/2079
4	H	0.29	0/1648	0.53	0/2246
4	J	0.29	0/1648	0.53	0/2246
4	L	0.29	0/1648	0.53	0/2246
All	All	0.28	0/21195	0.50	0/28782

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	2454	0	2403	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2454	0	2403	57	0
1	E	2454	0	2403	41	0
2	B	1353	0	1266	27	0
2	D	1353	0	1266	28	0
2	F	1353	0	1266	23	0
3	G	1502	0	1452	73	0
3	I	1502	0	1452	80	0
3	K	1502	0	1452	59	0
4	H	1608	0	1584	47	0
4	J	1608	0	1584	47	0
4	L	1608	0	1584	48	0
5	M	28	0	25	0	0
5	P	28	0	25	0	0
5	S	28	0	25	0	0
6	N	61	0	52	0	0
6	Q	61	0	52	0	0
6	T	61	0	52	2	0
7	O	94	0	79	2	0
7	R	94	0	79	0	0
7	U	94	0	79	1	0
8	A	28	0	26	1	0
8	B	14	0	13	1	0
8	C	28	0	26	1	0
8	D	14	0	13	1	0
8	E	28	0	26	1	0
8	F	14	0	13	1	0
All	All	21426	0	20700	538	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 13.

The worst 5 of 538 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:163:ASN:ND2	3:K:185:THR:O	2.12	0.80
3:K:17:ARG:HA	3:K:77:ILE:O	1.81	0.79
3:G:136:SER:HA	3:G:184:LEU:O	1.83	0.78
3:I:130:LEU:HA	3:I:188:LYS:HZ2	1.48	0.77
1:C:210:GLN:OE1	1:E:220:ARG:NE	2.14	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/345 (92%)	308 (98%)	8 (2%)	0	100	100
1	C	316/345 (92%)	309 (98%)	7 (2%)	0	100	100
1	E	316/345 (92%)	309 (98%)	7 (2%)	0	100	100
2	B	163/254 (64%)	151 (93%)	12 (7%)	0	100	100
2	D	163/254 (64%)	151 (93%)	12 (7%)	0	100	100
2	F	163/254 (64%)	151 (93%)	12 (7%)	0	100	100
3	G	196/219 (90%)	183 (93%)	13 (7%)	0	100	100
3	I	196/219 (90%)	185 (94%)	11 (6%)	0	100	100
3	K	196/219 (90%)	186 (95%)	10 (5%)	0	100	100
4	H	208/235 (88%)	194 (93%)	14 (7%)	0	100	100
4	J	208/235 (88%)	194 (93%)	14 (7%)	0	100	100
4	L	208/235 (88%)	194 (93%)	14 (7%)	0	100	100
All	All	2649/3159 (84%)	2515 (95%)	134 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/303 (92%)	278 (99%)	2 (1%)	81	86
1	C	280/303 (92%)	278 (99%)	2 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	280/303 (92%)	278 (99%)	2 (1%)	81	86
2	B	144/212 (68%)	144 (100%)	0	100	100
2	D	144/212 (68%)	144 (100%)	0	100	100
2	F	144/212 (68%)	144 (100%)	0	100	100
3	G	171/184 (93%)	171 (100%)	0	100	100
3	I	171/184 (93%)	171 (100%)	0	100	100
3	K	171/184 (93%)	169 (99%)	2 (1%)	67	78
4	H	180/200 (90%)	179 (99%)	1 (1%)	84	88
4	J	180/200 (90%)	179 (99%)	1 (1%)	84	88
4	L	180/200 (90%)	179 (99%)	1 (1%)	84	88
All	All	2325/2697 (86%)	2314 (100%)	11 (0%)	85	90

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	202	GLN
3	K	91	GLN
4	L	202	GLN
3	K	216	ARG
1	E	191	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	6	GLN
3	G	91	GLN
3	I	91	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

45 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	0.38	0	17,19,21	0.51	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	N	1	6,1	14,14,15	0.41	0	17,19,21	0.44	0
6	NAG	N	2	6	14,14,15	0.18	0	17,19,21	0.50	0
6	BMA	N	3	6	11,11,12	0.52	0	15,15,17	0.94	0
6	MAN	N	4	6	11,11,12	0.66	0	15,15,17	0.88	1 (6%)
6	MAN	N	5	6	11,11,12	0.81	1 (9%)	15,15,17	0.83	1 (6%)
7	NAG	O	1	7,1	14,14,15	0.42	0	17,19,21	0.37	0
7	NAG	O	2	7	14,14,15	0.22	0	17,19,21	0.73	0
7	BMA	O	3	7	11,11,12	0.79	0	15,15,17	1.01	0
7	MAN	O	4	7	11,11,12	1.19	1 (9%)	15,15,17	1.70	3 (20%)
7	MAN	O	5	7	11,11,12	0.67	0	15,15,17	0.93	1 (6%)
7	MAN	O	6	7	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
7	MAN	O	7	7	11,11,12	1.05	1 (9%)	15,15,17	0.84	1 (6%)
7	MAN	O	8	7	11,11,12	1.02	1 (9%)	15,15,17	0.91	1 (6%)
5	NAG	P	1	5,1	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	P	2	5	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	Q	1	6,1	14,14,15	0.41	0	17,19,21	0.43	0
6	NAG	Q	2	6	14,14,15	0.19	0	17,19,21	0.50	0
6	BMA	Q	3	6	11,11,12	0.52	0	15,15,17	0.94	0
6	MAN	Q	4	6	11,11,12	0.66	0	15,15,17	0.88	1 (6%)
6	MAN	Q	5	6	11,11,12	0.81	1 (9%)	15,15,17	0.83	1 (6%)
7	NAG	R	1	7,1	14,14,15	0.42	0	17,19,21	0.37	0
7	NAG	R	2	7	14,14,15	0.22	0	17,19,21	0.73	0
7	BMA	R	3	7	11,11,12	0.79	0	15,15,17	1.01	0
7	MAN	R	4	7	11,11,12	1.20	1 (9%)	15,15,17	1.70	3 (20%)
7	MAN	R	5	7	11,11,12	0.65	0	15,15,17	0.93	1 (6%)
7	MAN	R	6	7	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
7	MAN	R	7	7	11,11,12	1.06	1 (9%)	15,15,17	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	R	8	7	11,11,12	1.01	1 (9%)	15,15,17	0.91	1 (6%)
5	NAG	S	1	5,1	14,14,15	0.36	0	17,19,21	0.52	0
5	NAG	S	2	5	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	T	1	6,1	14,14,15	0.40	0	17,19,21	0.44	0
6	NAG	T	2	6	14,14,15	0.20	0	17,19,21	0.50	0
6	BMA	T	3	6	11,11,12	0.53	0	15,15,17	0.94	0
6	MAN	T	4	6	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
6	MAN	T	5	6	11,11,12	0.80	1 (9%)	15,15,17	0.83	1 (6%)
7	NAG	U	1	7,1	14,14,15	0.42	0	17,19,21	0.37	0
7	NAG	U	2	7	14,14,15	0.23	0	17,19,21	0.73	0
7	BMA	U	3	7	11,11,12	0.79	0	15,15,17	1.01	0
7	MAN	U	4	7	11,11,12	1.20	1 (9%)	15,15,17	1.70	3 (20%)
7	MAN	U	5	7	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
7	MAN	U	6	7	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
7	MAN	U	7	7	11,11,12	1.05	1 (9%)	15,15,17	0.84	1 (6%)
7	MAN	U	8	7	11,11,12	1.02	1 (9%)	15,15,17	0.92	1 (6%)

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	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	2/2/19/22	0/1/1/1
6	MAN	N	5	6	-	1/2/19/22	0/1/1/1
7	NAG	O	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	2/2/19/22	0/1/1/1
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
7	MAN	O	5	7	-	0/2/19/22	0/1/1/1
7	MAN	O	6	7	-	0/2/19/22	0/1/1/1
7	MAN	O	7	7	-	2/2/19/22	0/1/1/1
7	MAN	O	8	7	-	1/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	1/2/19/22	0/1/1/1
7	NAG	R	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	R	2	7	-	2/6/23/26	0/1/1/1
7	BMA	R	3	7	-	2/2/19/22	0/1/1/1
7	MAN	R	4	7	-	0/2/19/22	0/1/1/1
7	MAN	R	5	7	-	0/2/19/22	0/1/1/1
7	MAN	R	6	7	-	0/2/19/22	0/1/1/1
7	MAN	R	7	7	-	2/2/19/22	0/1/1/1
7	MAN	R	8	7	-	1/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	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
6	MAN	T	4	6	-	2/2/19/22	0/1/1/1
6	MAN	T	5	6	-	1/2/19/22	0/1/1/1
7	NAG	U	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	U	2	7	-	2/6/23/26	0/1/1/1
7	BMA	U	3	7	-	2/2/19/22	0/1/1/1
7	MAN	U	4	7	-	0/2/19/22	0/1/1/1
7	MAN	U	5	7	-	0/2/19/22	0/1/1/1
7	MAN	U	6	7	-	0/2/19/22	0/1/1/1
7	MAN	U	7	7	-	2/2/19/22	0/1/1/1
7	MAN	U	8	7	-	1/2/19/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	4	MAN	O5-C1	-3.42	1.37	1.43
7	U	4	MAN	O5-C1	-3.41	1.38	1.43
7	O	4	MAN	O5-C1	-3.41	1.38	1.43
7	R	7	MAN	O5-C1	-3.23	1.38	1.43
7	U	7	MAN	O5-C1	-3.22	1.38	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	4	MAN	C3-C4-C5	-3.69	103.54	110.23
7	U	4	MAN	C3-C4-C5	-3.69	103.54	110.23
7	O	4	MAN	C3-C4-C5	-3.68	103.55	110.23
7	R	4	MAN	C1-C2-C3	-3.09	105.15	109.64
7	U	4	MAN	C1-C2-C3	-3.07	105.17	109.64

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

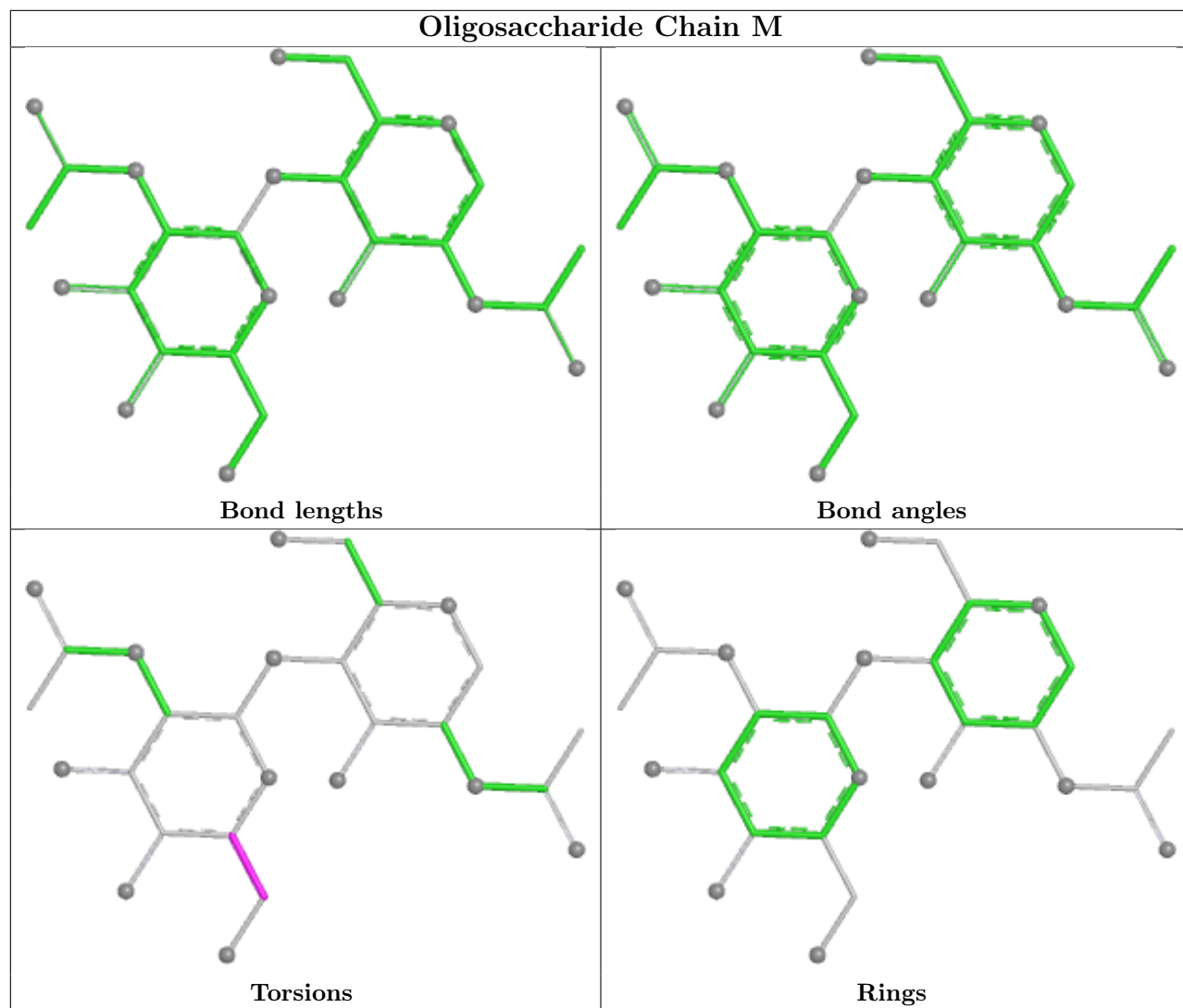
Mol	Chain	Res	Type	Atoms
7	O	7	MAN	O5-C5-C6-O6
7	R	7	MAN	O5-C5-C6-O6
7	U	7	MAN	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6

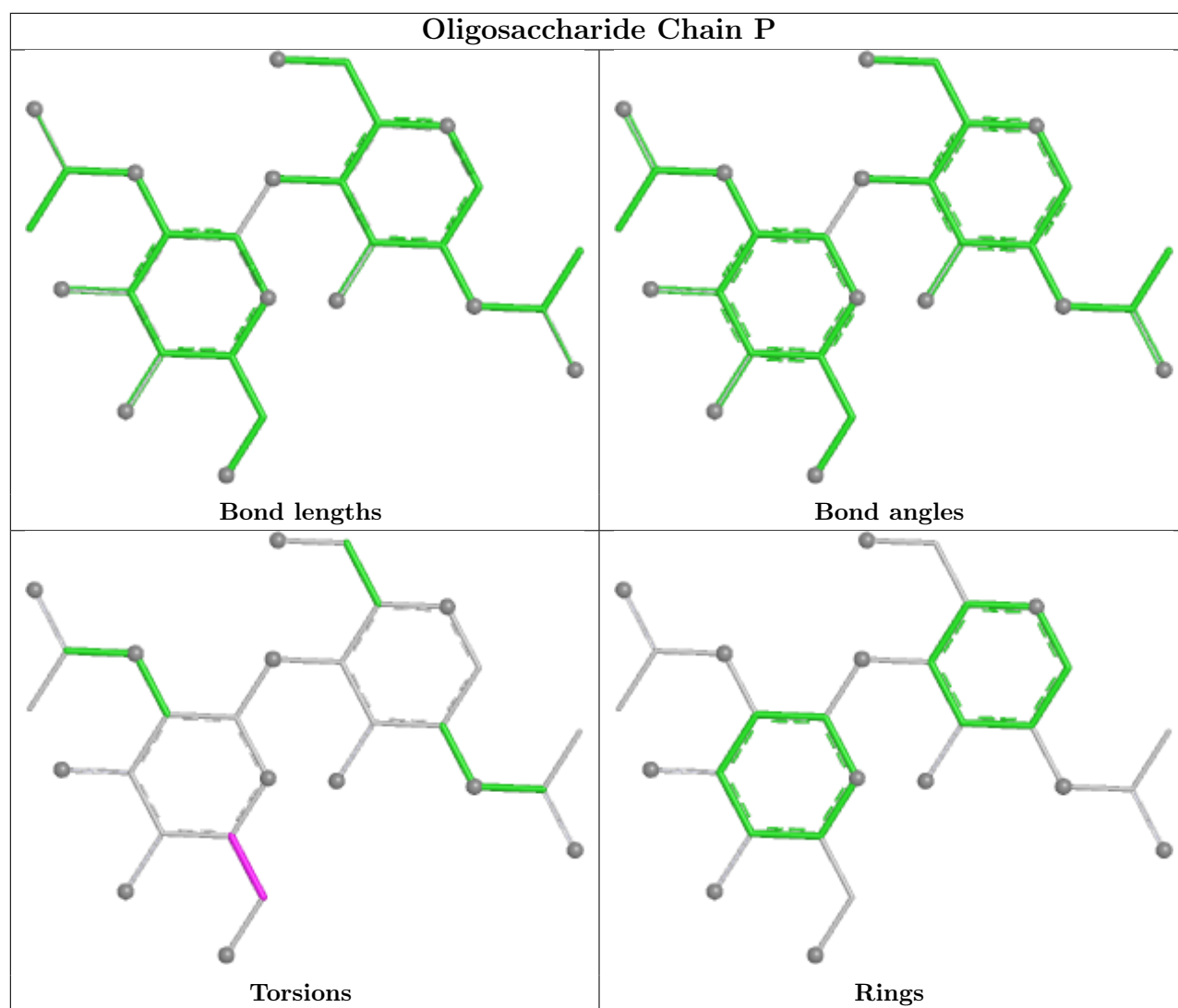
There are no ring outliers.

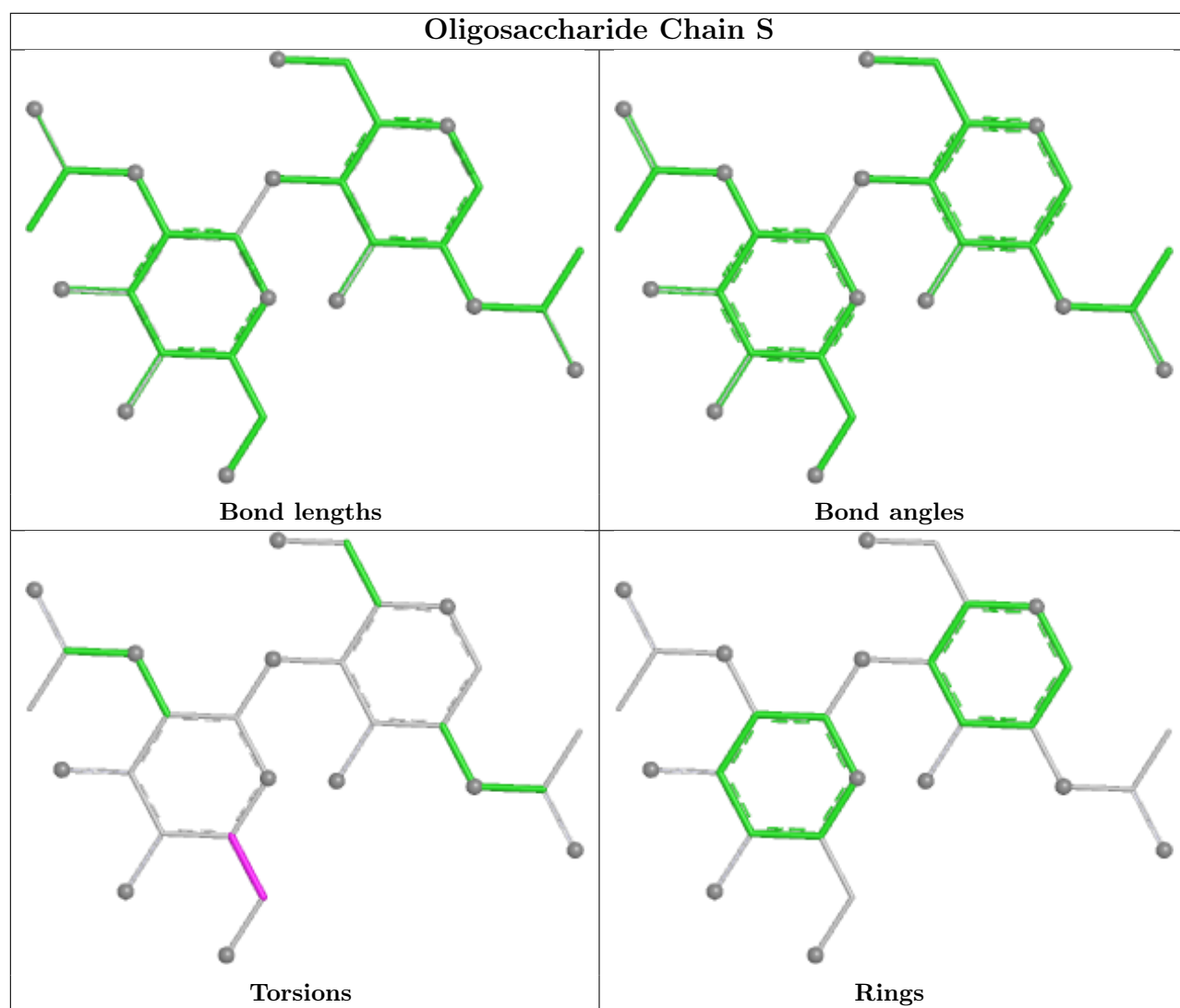
4 monomers are involved in 5 short contacts:

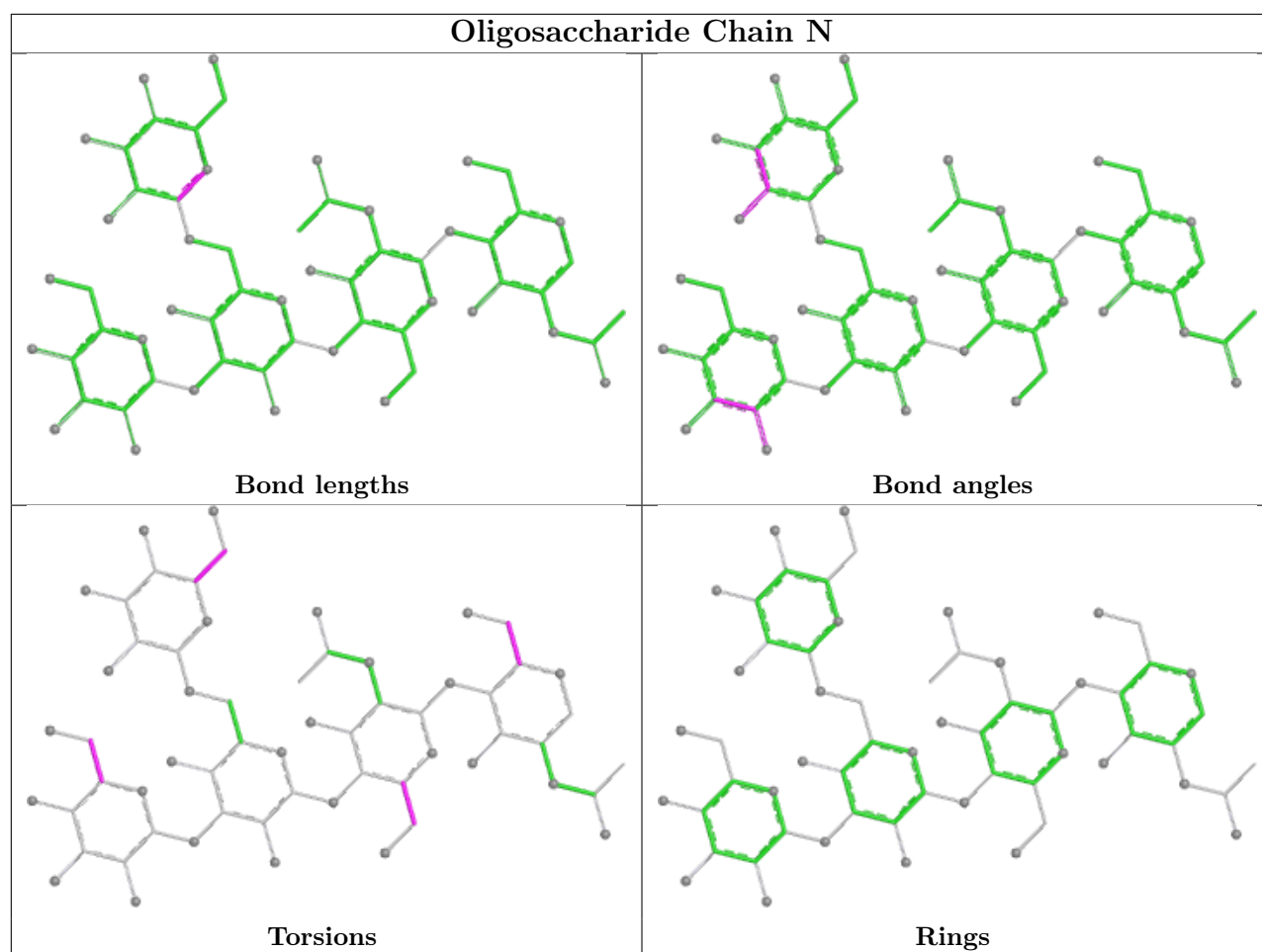
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	2	NAG	1	0
6	T	3	BMA	1	0
7	U	6	MAN	1	0
7	O	6	MAN	2	0

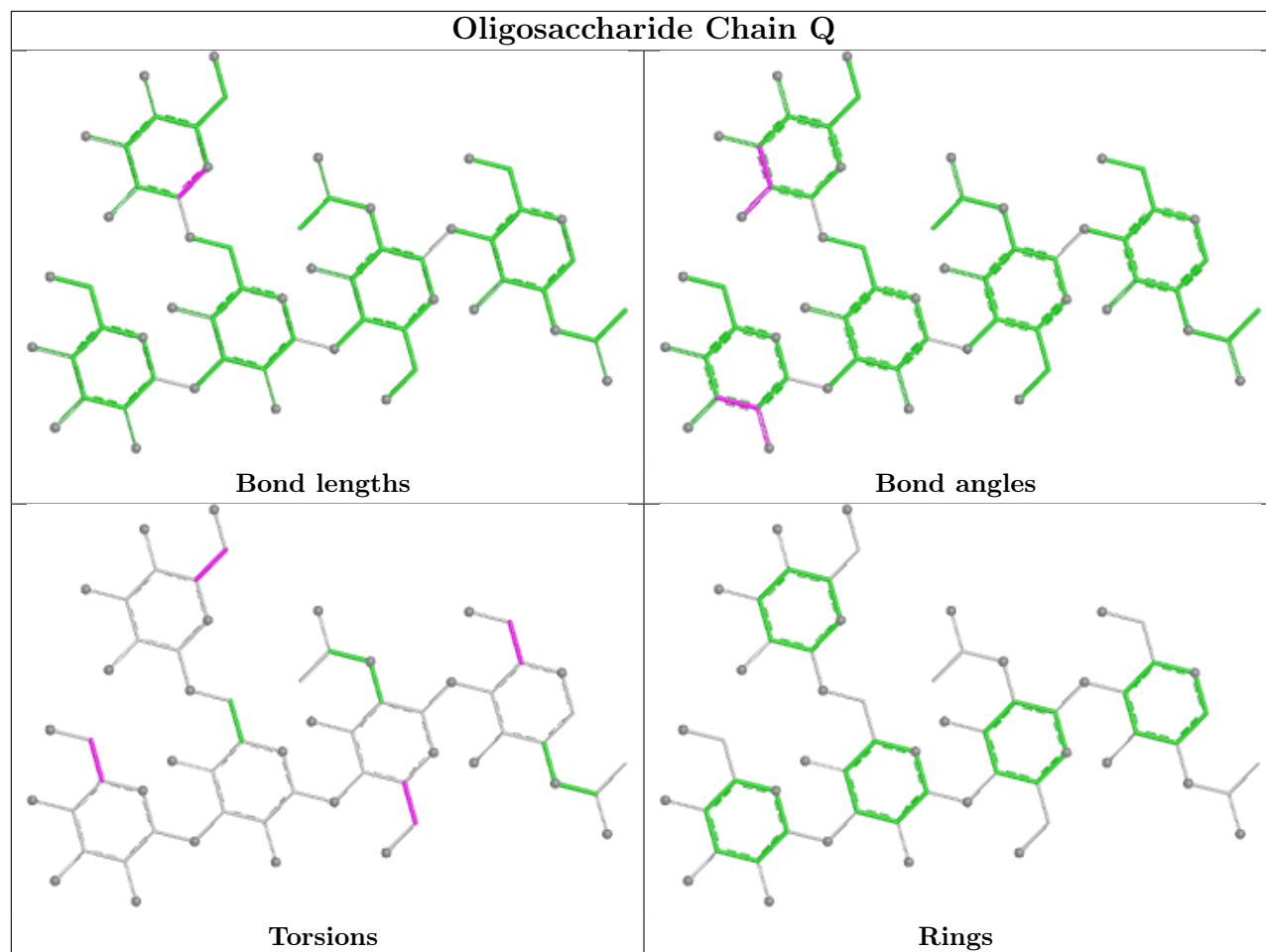
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

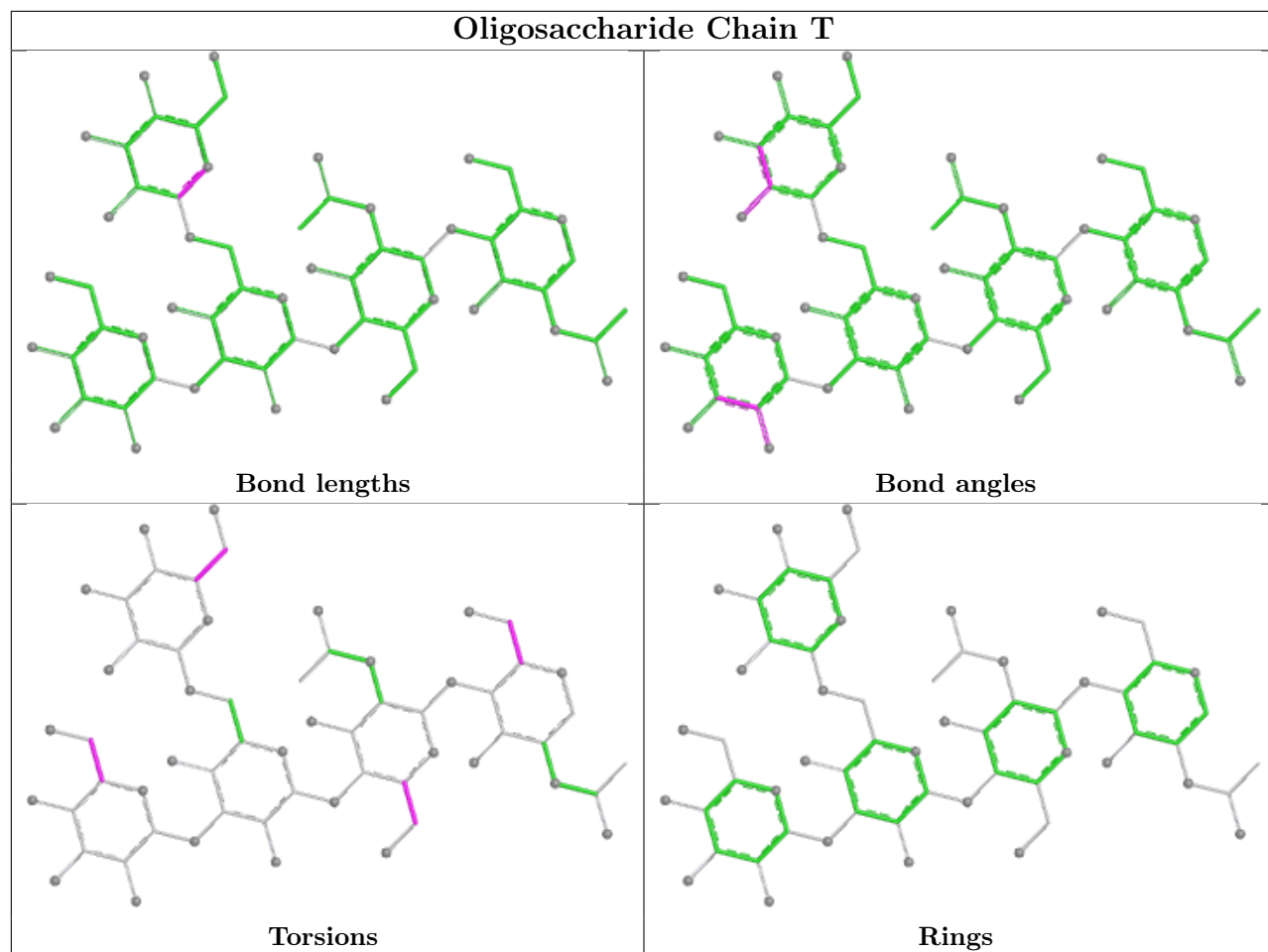


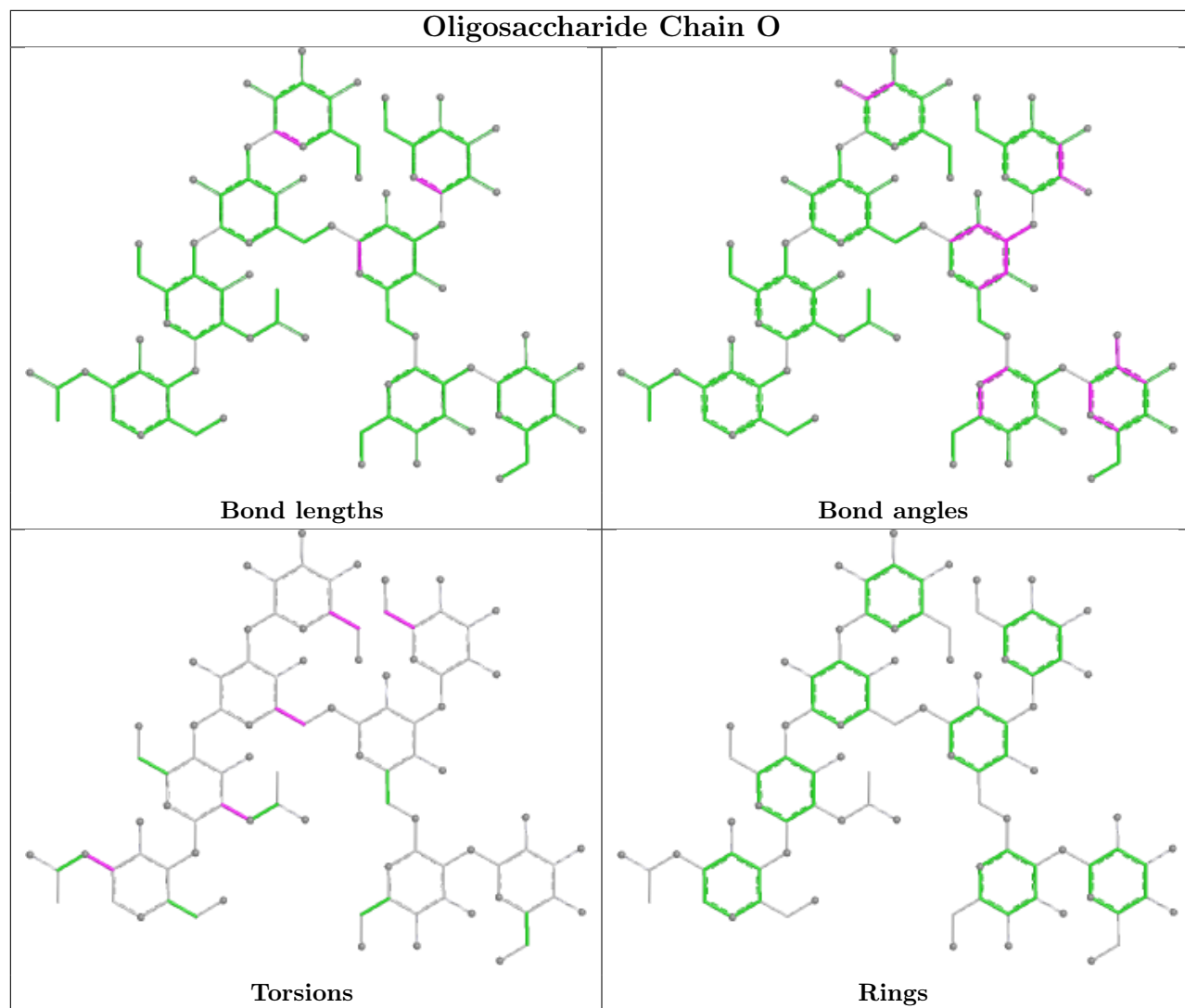


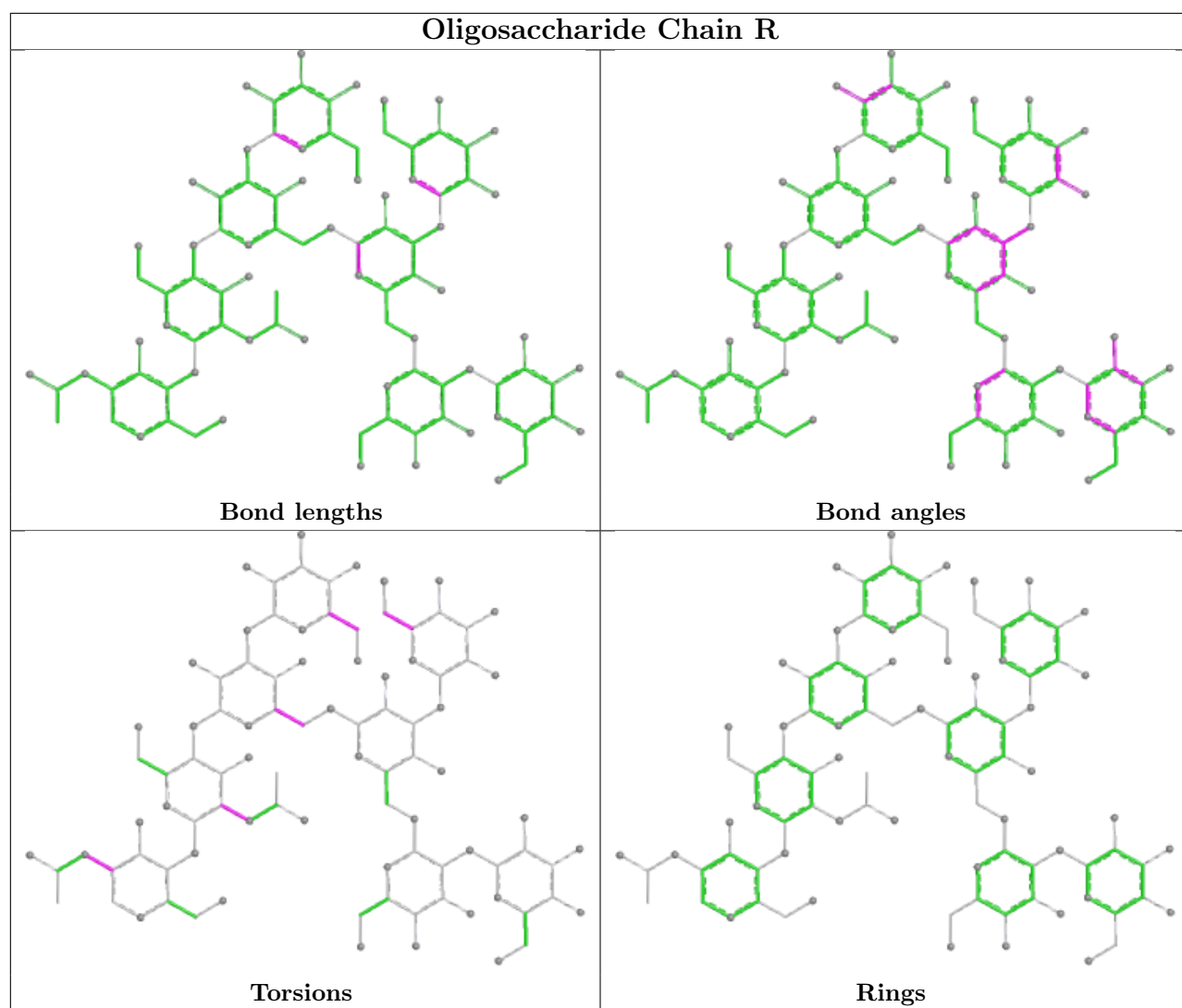


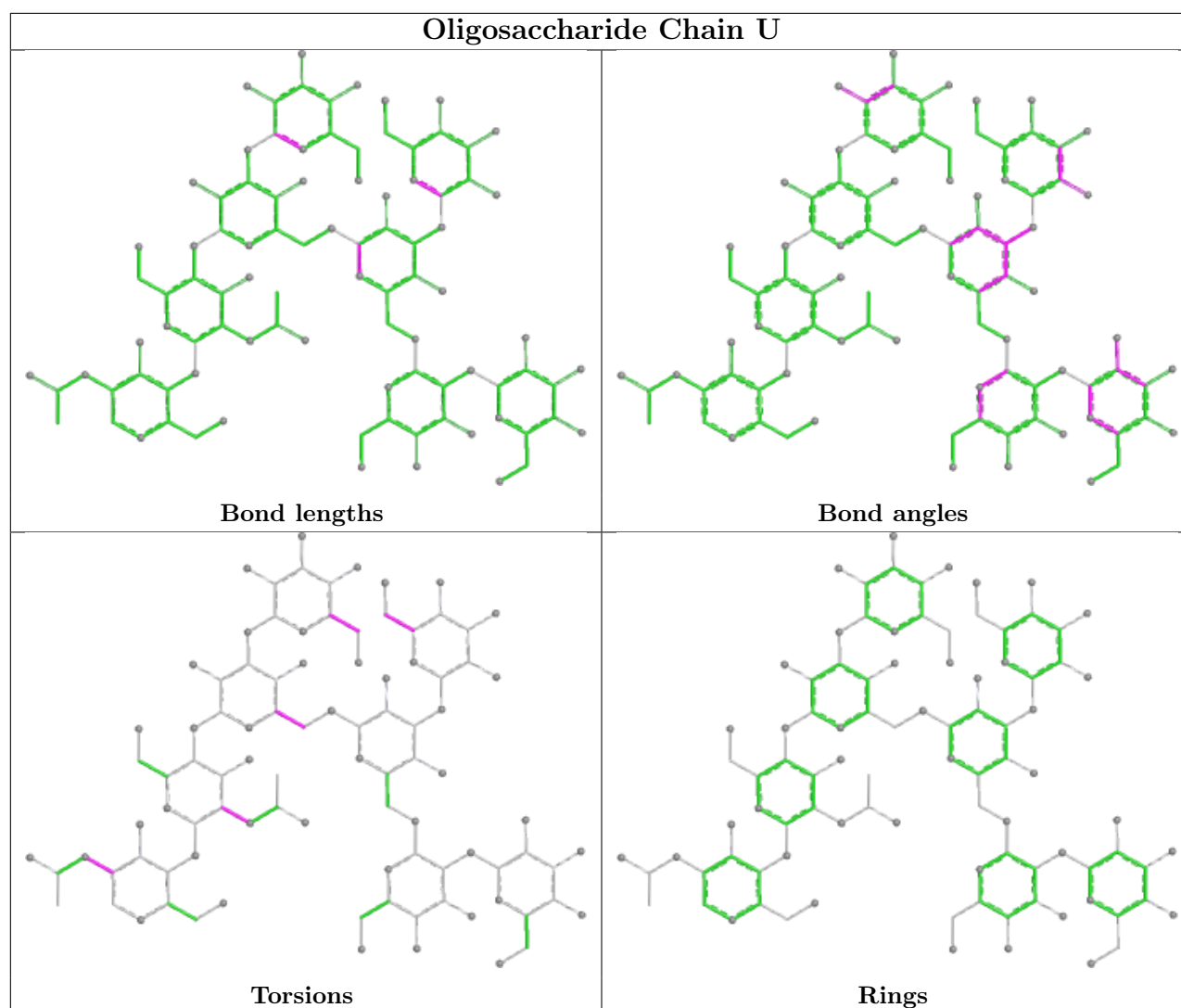












5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	B	301	2	14,14,15	0.43	0	17,19,21	1.35	2 (11%)
8	NAG	E	402	1	14,14,15	0.20	0	17,19,21	0.49	0
8	NAG	D	301	2	14,14,15	0.44	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	402	1	14,14,15	0.19	0	17,19,21	0.49	0
8	NAG	C	402	1	14,14,15	0.20	0	17,19,21	0.49	0
8	NAG	F	301	2	14,14,15	0.43	0	17,19,21	1.37	2 (11%)
8	NAG	A	401	1	14,14,15	0.33	0	17,19,21	0.51	0
8	NAG	E	401	1	14,14,15	0.33	0	17,19,21	0.52	0
8	NAG	C	401	1	14,14,15	0.34	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	301	2	-	6/6/23/26	0/1/1/1
8	NAG	E	402	1	-	2/6/23/26	0/1/1/1
8	NAG	D	301	2	-	6/6/23/26	0/1/1/1
8	NAG	A	402	1	-	2/6/23/26	0/1/1/1
8	NAG	C	402	1	-	2/6/23/26	0/1/1/1
8	NAG	F	301	2	-	6/6/23/26	0/1/1/1
8	NAG	A	401	1	-	4/6/23/26	0/1/1/1
8	NAG	E	401	1	-	4/6/23/26	0/1/1/1
8	NAG	C	401	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	301	NAG	C2-N2-C7	4.66	129.15	122.90
8	D	301	NAG	C2-N2-C7	4.62	129.09	122.90
8	B	301	NAG	C2-N2-C7	4.59	129.05	122.90
8	D	301	NAG	C1-C2-N2	2.33	114.11	110.43
8	F	301	NAG	C1-C2-N2	2.31	114.08	110.43

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	401	NAG	O5-C5-C6-O6
8	C	401	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	E	401	NAG	O5-C5-C6-O6
8	A	402	NAG	O5-C5-C6-O6
8	C	402	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	301	NAG	1	0
8	D	301	NAG	1	0
8	F	301	NAG	1	0
8	A	401	NAG	1	0
8	E	401	NAG	1	0
8	C	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

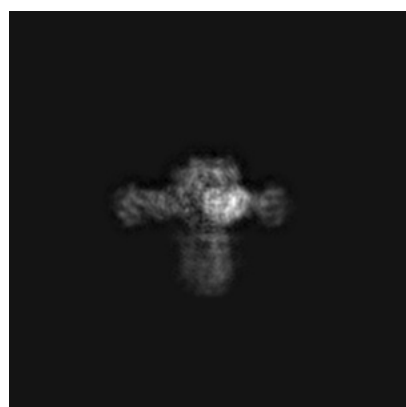
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22654. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

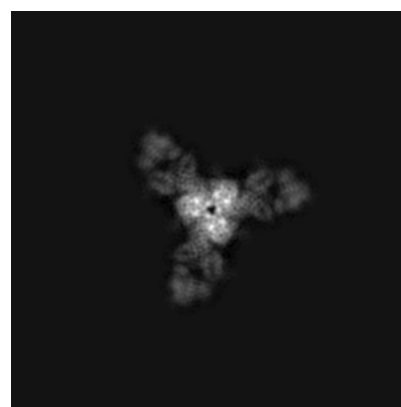
6.1.1 Primary map



X



Y

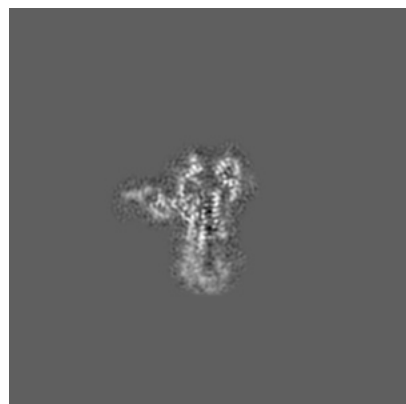


Z

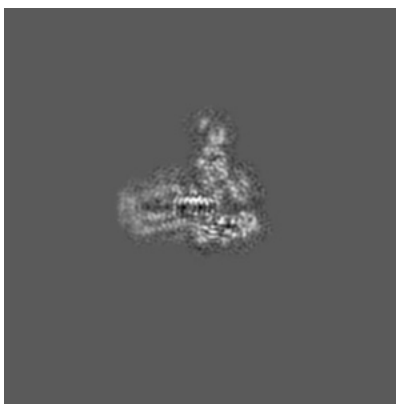
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

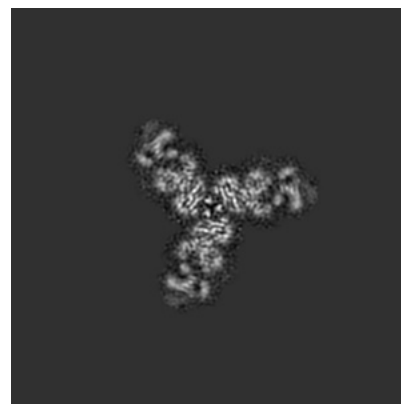
6.2.1 Primary map



X Index: 150



Y Index: 150

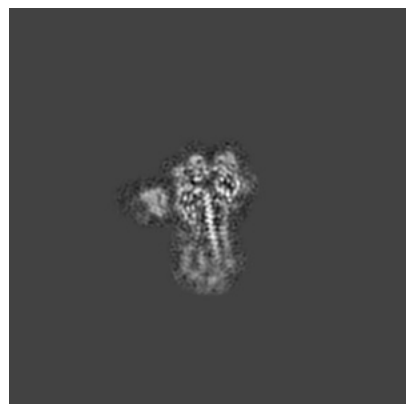


Z Index: 150

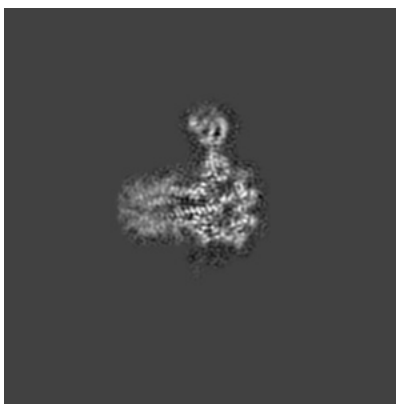
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 155



Y Index: 156

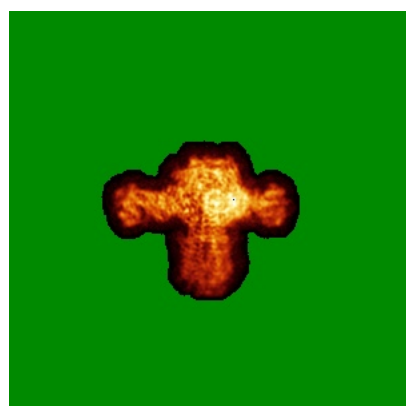


Z Index: 156

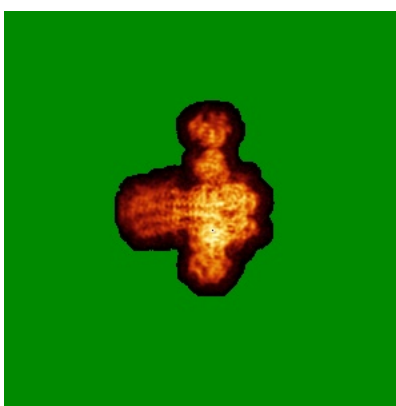
The images above show the largest variance slices of the map in three orthogonal directions.

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

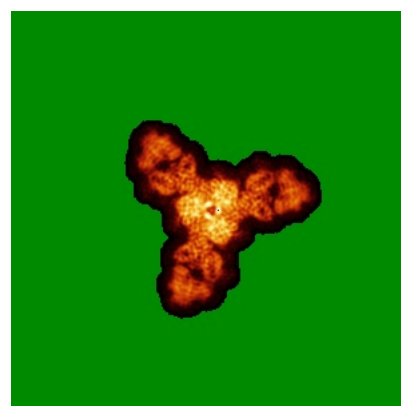
6.4.1 Primary map



X



Y

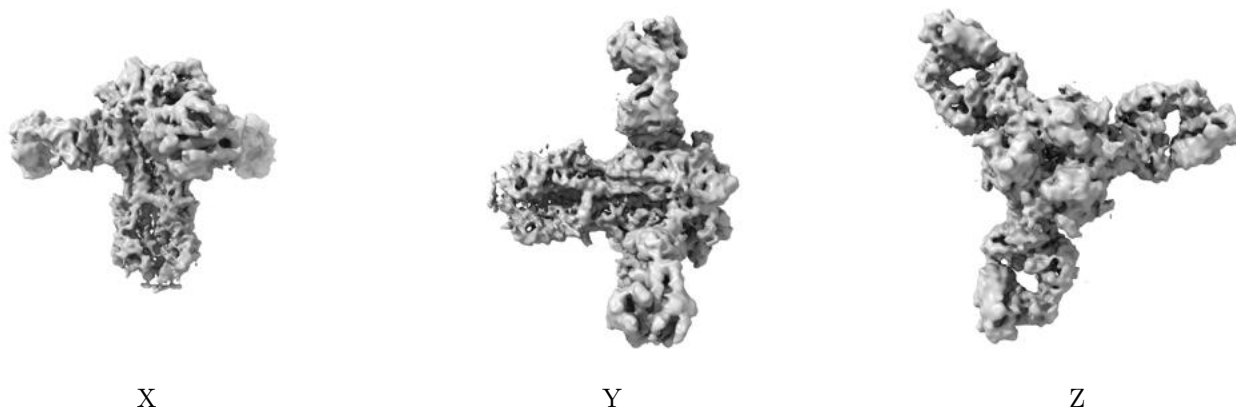


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

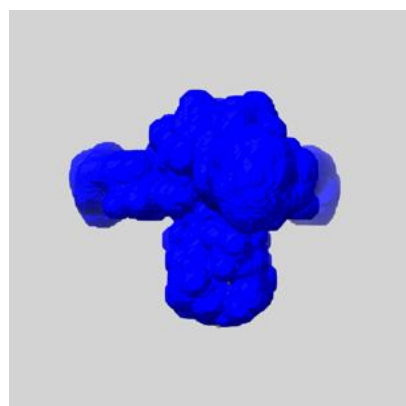
6.6 Mask visualisation [i](#)

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

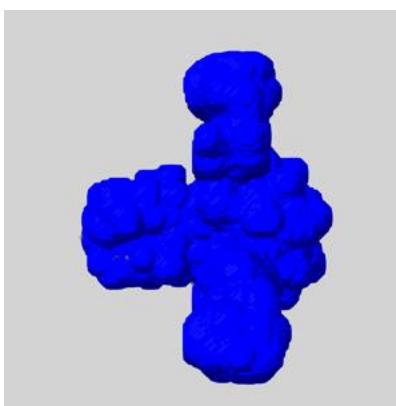
A mask typically either:

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

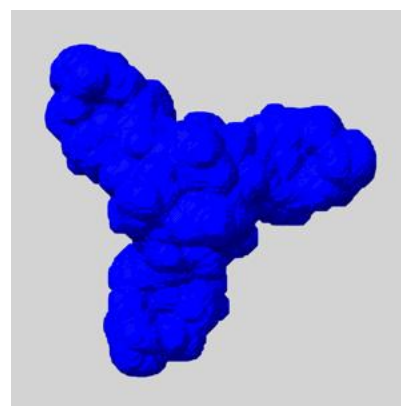
6.6.1 emd_22654_msk_1.map [i](#)



X



Y

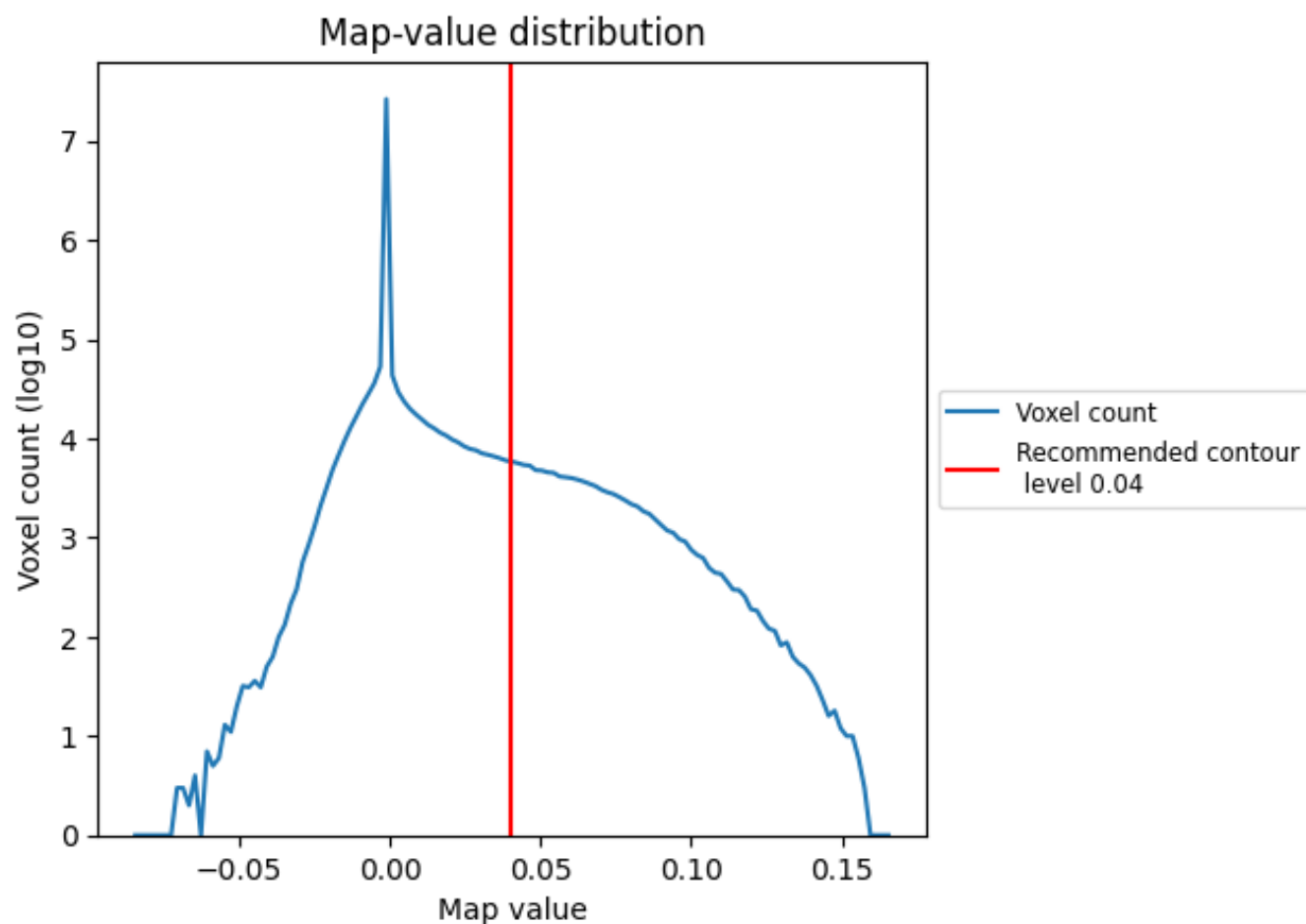


Z

7 Map analysis [i](#)

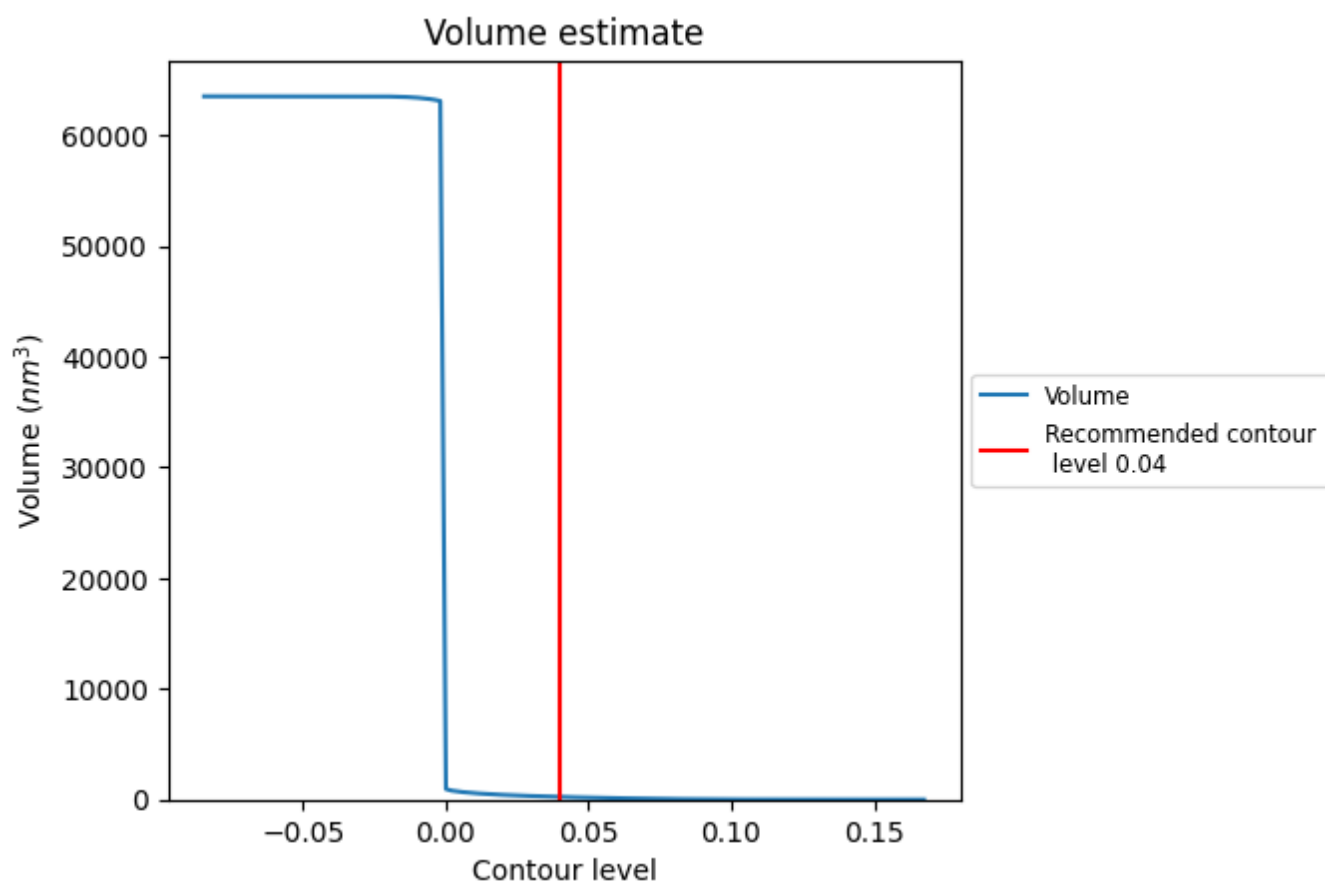
This section contains the results of statistical analysis of the map.

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.

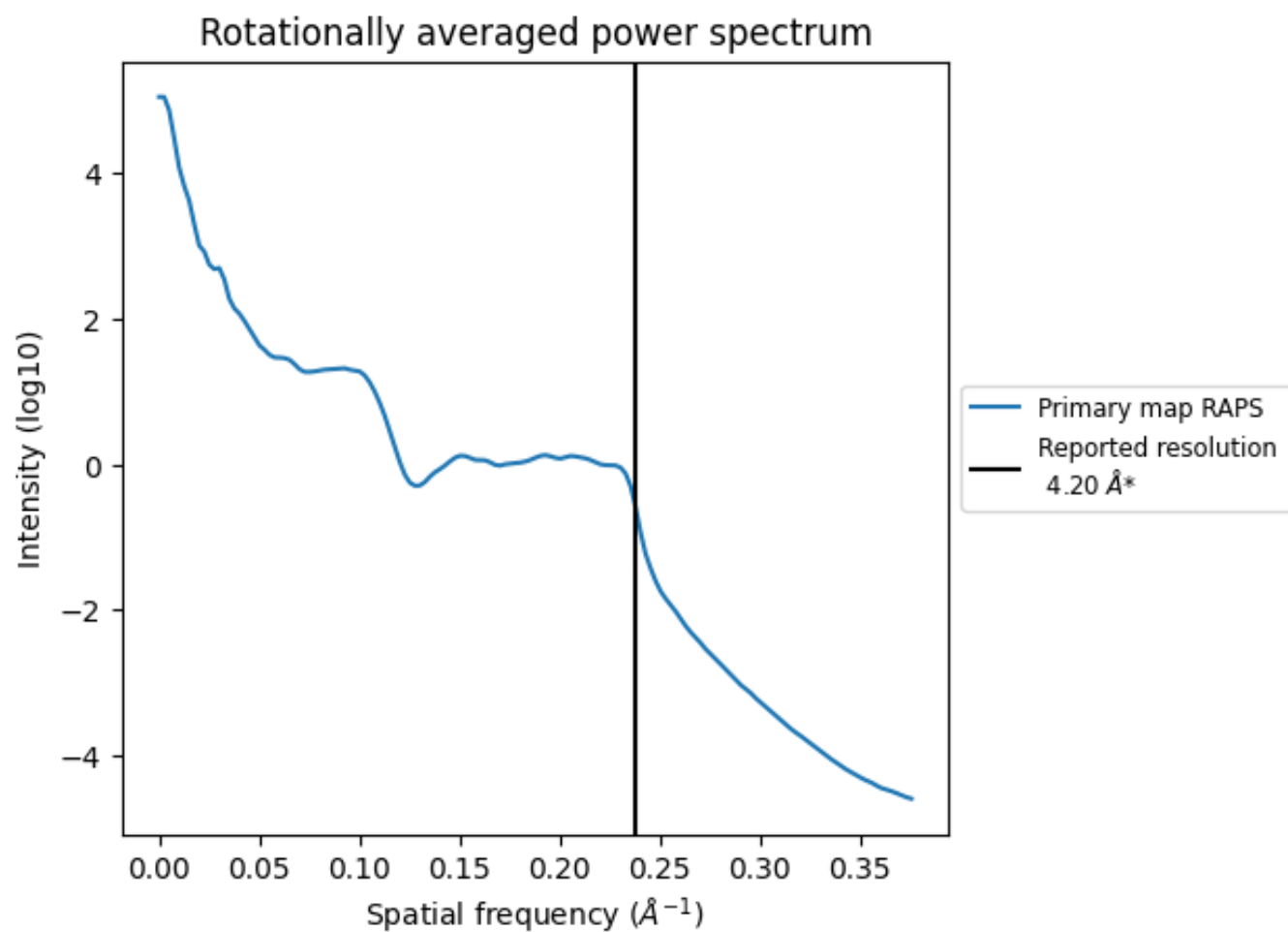
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 219 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

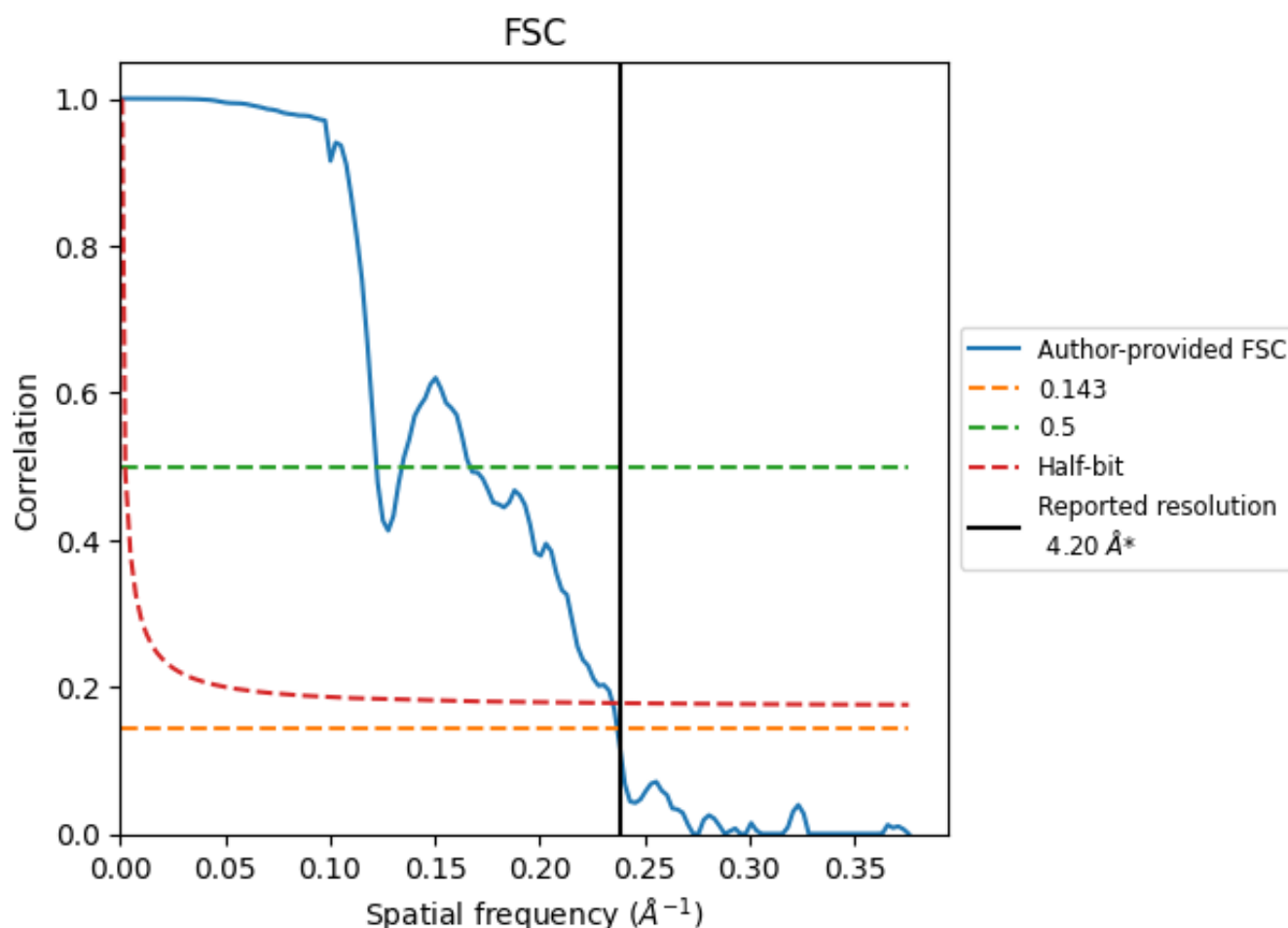


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

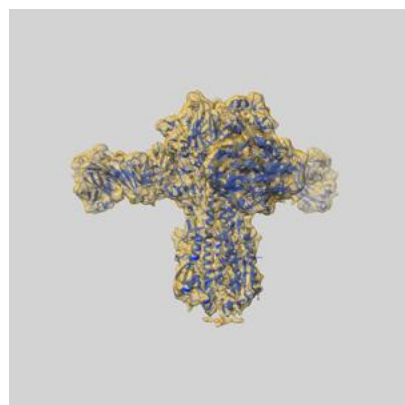
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	8.18	4.26
Unmasked-calculated*	-	-	-

*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-22654 and PDB model 7K3A. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

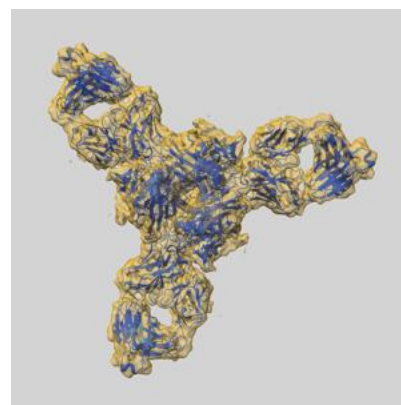
9.1 Map-model overlay [i](#)



X



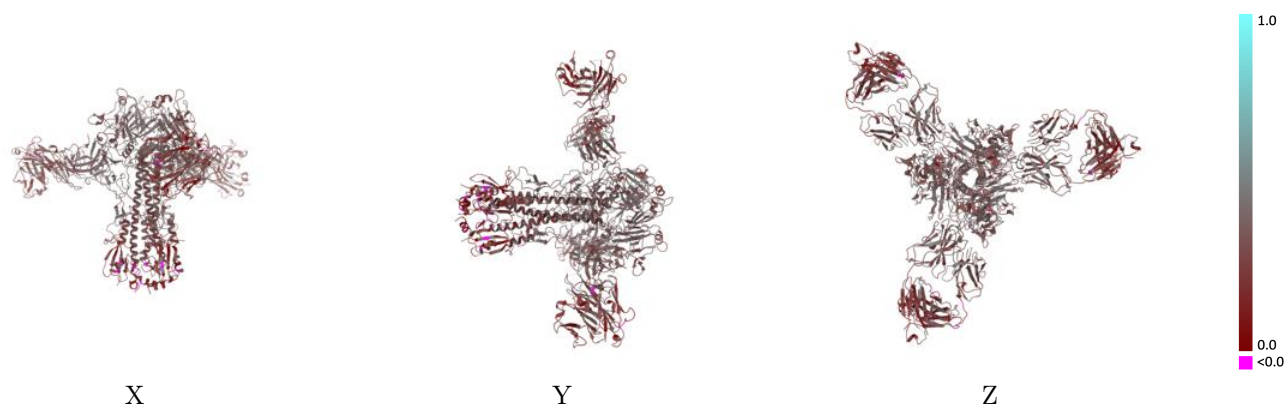
Y



Z

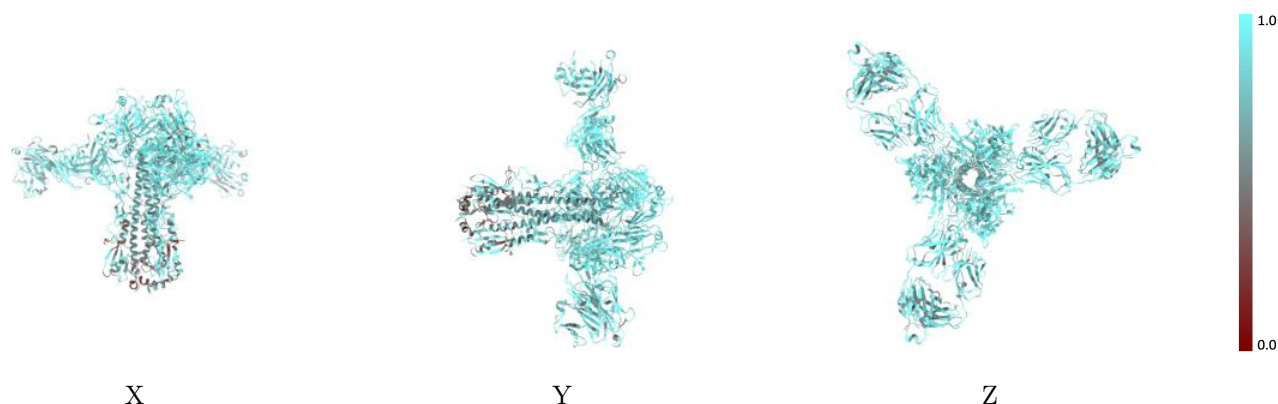
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



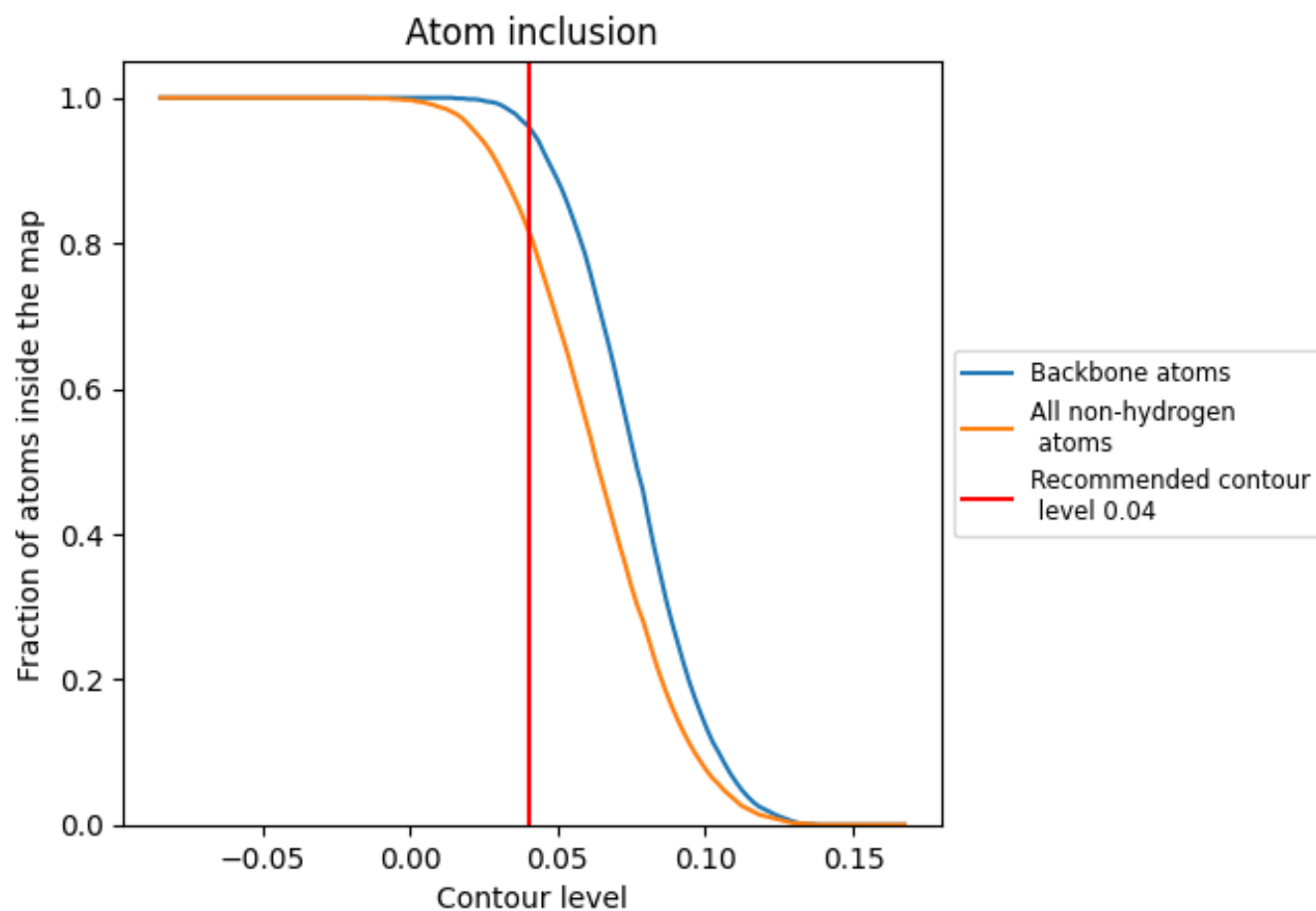
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.3210
A	 0.8780	 0.3660
B	 0.6630	 0.2680
C	 0.8820	 0.3680
D	 0.6500	 0.2560
E	 0.8820	 0.3680
F	 0.6620	 0.2650
G	 0.8440	 0.2900
H	 0.8440	 0.3240
I	 0.8410	 0.2840
J	 0.8430	 0.3240
K	 0.8490	 0.2910
L	 0.8430	 0.3220
M	 0.2860	 0.2630
N	 0.8530	 0.3620
O	 0.7230	 0.3590
P	 0.3210	 0.2580
Q	 0.8530	 0.3570
R	 0.7770	 0.3830
S	 0.3210	 0.2820
T	 0.8530	 0.3610
U	 0.7770	 0.3920

