



## Full wwPDB EM Validation Report ⓘ

Dec 26, 2024 – 03:36 PM EST

PDB ID : 6U5S  
EMDB ID : EMD-20654  
Title : NTD of GluA2 in complex with CNIH3 - with antagonist ZK200775 - in pseudo-symmetric global conformation  
Authors : Nakagawa, T.  
Deposited on : 2019-08-28  
Resolution : 3.07 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>.

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

EMDB validation analysis : 0.0.1.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) : 2.40

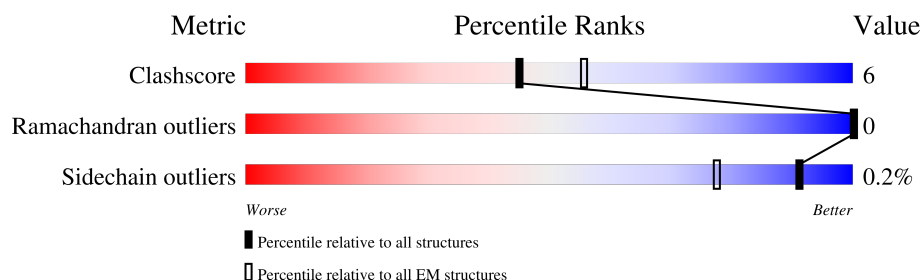
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.07 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	889	
1	B	889	
1	C	889	
1	D	889	
2	E	2	
2	G	2	
2	I	2	
2	K	2	

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Mol	Chain	Length	Quality of chain
3	F	3	<div><div></div><div>67%</div><div>33%</div><div>67%</div></div>
3	H	3	<div><div></div><div>67%</div><div>33%</div><div>67%</div></div>
3	J	3	<div><div></div><div>67%</div><div>33%</div><div>67%</div></div>
3	L	3	<div><div></div><div>33%</div><div>33%</div><div>67%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21509 atoms, of which 9803 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	376	Total	C	H	N	O	S	0	0
			5176	1804	2366	475	522	9		
1	B	376	Total	C	H	N	O	S	0	0
			5357	1847	2468	491	542	9		
1	C	376	Total	C	H	N	O	S	0	0
			5292	1823	2442	476	542	9		
1	D	376	Total	C	H	N	O	S	0	0
			5368	1847	2479	491	542	9		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	ARG	GLN	conflict	UNP P19491
A	854	ASP	-	expression tag	UNP P19491
A	855	TYR	-	expression tag	UNP P19491
A	856	LYS	-	expression tag	UNP P19491
A	857	ASP	-	expression tag	UNP P19491
A	858	ASP	-	expression tag	UNP P19491
A	859	ASP	-	expression tag	UNP P19491
A	860	ASP	-	expression tag	UNP P19491
A	861	LYS	-	expression tag	UNP P19491
A	862	GLU	-	expression tag	UNP P19491
A	863	GLY	-	expression tag	UNP P19491
A	864	TYR	-	expression tag	UNP P19491
A	865	ASN	-	expression tag	UNP P19491
A	866	VAL	-	expression tag	UNP P19491
A	867	TYR	-	expression tag	UNP P19491
A	868	GLY	-	expression tag	UNP P19491
A	869	ILE	-	expression tag	UNP P19491
A	870	GLU	-	expression tag	UNP P19491
A	871	SER	-	expression tag	UNP P19491
A	872	VAL	-	expression tag	UNP P19491
A	873	LYS	-	expression tag	UNP P19491
A	874	ILE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	592	ARG	GLN	conflict	UNP P19491
B	854	ASP	-	expression tag	UNP P19491
B	855	TYR	-	expression tag	UNP P19491
B	856	LYS	-	expression tag	UNP P19491
B	857	ASP	-	expression tag	UNP P19491
B	858	ASP	-	expression tag	UNP P19491
B	859	ASP	-	expression tag	UNP P19491
B	860	ASP	-	expression tag	UNP P19491
B	861	LYS	-	expression tag	UNP P19491
B	862	GLU	-	expression tag	UNP P19491
B	863	GLY	-	expression tag	UNP P19491
B	864	TYR	-	expression tag	UNP P19491
B	865	ASN	-	expression tag	UNP P19491
B	866	VAL	-	expression tag	UNP P19491
B	867	TYR	-	expression tag	UNP P19491
B	868	GLY	-	expression tag	UNP P19491
B	869	ILE	-	expression tag	UNP P19491
B	870	GLU	-	expression tag	UNP P19491
B	871	SER	-	expression tag	UNP P19491
B	872	VAL	-	expression tag	UNP P19491
B	873	LYS	-	expression tag	UNP P19491
B	874	ILE	-	expression tag	UNP P19491
C	592	ARG	GLN	conflict	UNP P19491
C	854	ASP	-	expression tag	UNP P19491
C	855	TYR	-	expression tag	UNP P19491
C	856	LYS	-	expression tag	UNP P19491
C	857	ASP	-	expression tag	UNP P19491
C	858	ASP	-	expression tag	UNP P19491
C	859	ASP	-	expression tag	UNP P19491
C	860	ASP	-	expression tag	UNP P19491
C	861	LYS	-	expression tag	UNP P19491
C	862	GLU	-	expression tag	UNP P19491
C	863	GLY	-	expression tag	UNP P19491
C	864	TYR	-	expression tag	UNP P19491
C	865	ASN	-	expression tag	UNP P19491
C	866	VAL	-	expression tag	UNP P19491
C	867	TYR	-	expression tag	UNP P19491
C	868	GLY	-	expression tag	UNP P19491
C	869	ILE	-	expression tag	UNP P19491
C	870	GLU	-	expression tag	UNP P19491
C	871	SER	-	expression tag	UNP P19491
C	872	VAL	-	expression tag	UNP P19491

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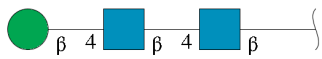
Chain	Residue	Modelled	Actual	Comment	Reference
C	873	LYS	-	expression tag	UNP P19491
C	874	ILE	-	expression tag	UNP P19491
D	592	ARG	GLN	conflict	UNP P19491
D	854	ASP	-	expression tag	UNP P19491
D	855	TYR	-	expression tag	UNP P19491
D	856	LYS	-	expression tag	UNP P19491
D	857	ASP	-	expression tag	UNP P19491
D	858	ASP	-	expression tag	UNP P19491
D	859	ASP	-	expression tag	UNP P19491
D	860	ASP	-	expression tag	UNP P19491
D	861	LYS	-	expression tag	UNP P19491
D	862	GLU	-	expression tag	UNP P19491
D	863	GLY	-	expression tag	UNP P19491
D	864	TYR	-	expression tag	UNP P19491
D	865	ASN	-	expression tag	UNP P19491
D	866	VAL	-	expression tag	UNP P19491
D	867	TYR	-	expression tag	UNP P19491
D	868	GLY	-	expression tag	UNP P19491
D	869	ILE	-	expression tag	UNP P19491
D	870	GLU	-	expression tag	UNP P19491
D	871	SER	-	expression tag	UNP P19491
D	872	VAL	-	expression tag	UNP P19491
D	873	LYS	-	expression tag	UNP P19491
D	874	ILE	-	expression tag	UNP P19491

- Molecule 2 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	
2	E	2	Total 40	C 16	H 12	N 2	O 10	0	0
2	G	2	Total 40	C 16	H 12	N 2	O 10	0	0
2	I	2	Total 40	C 16	H 12	N 2	O 10	0	0
2	K	2	Total 40	C 16	H 12	N 2	O 10	0	0

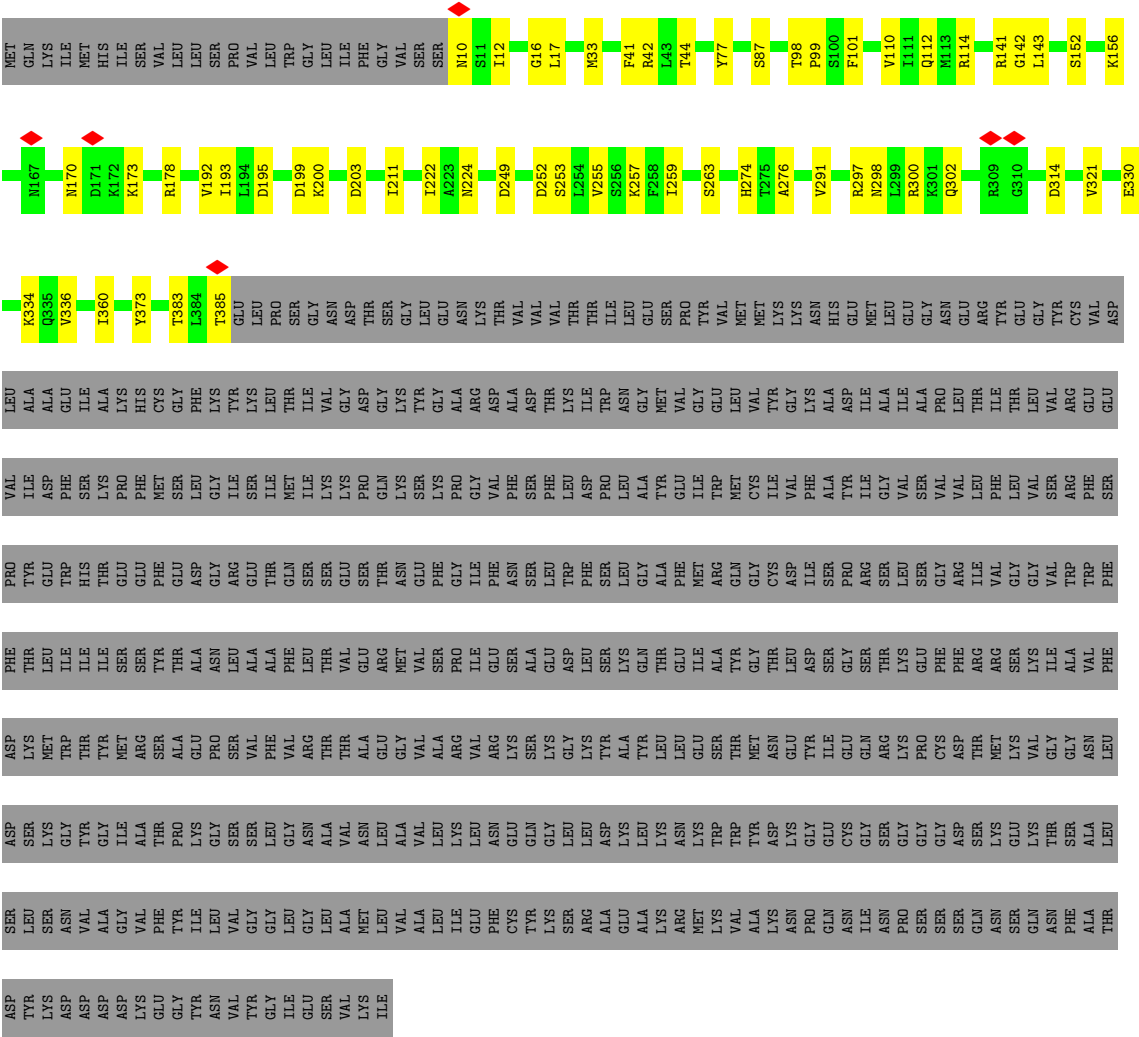
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



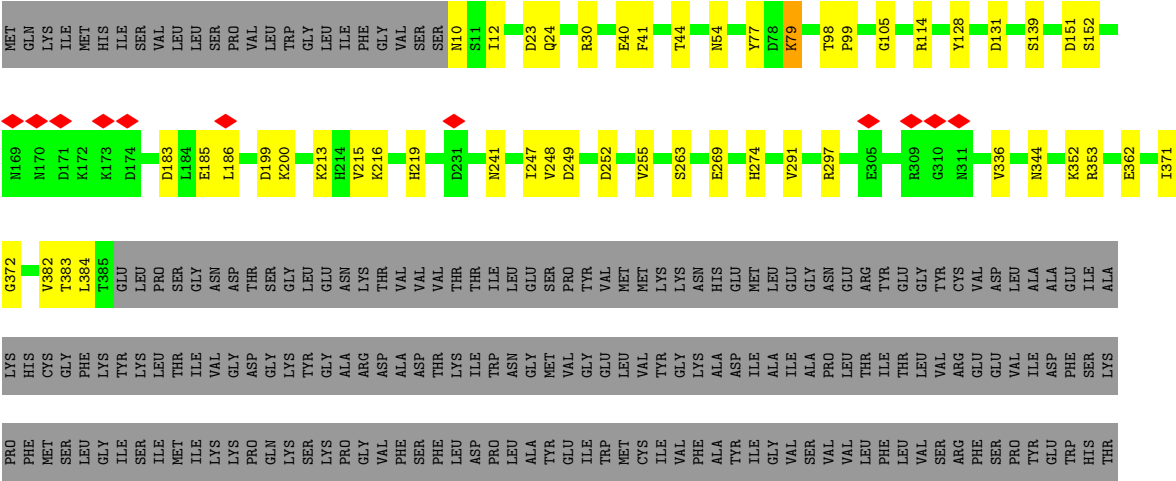
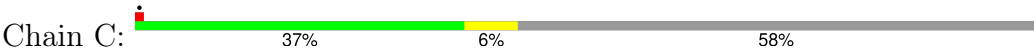
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		





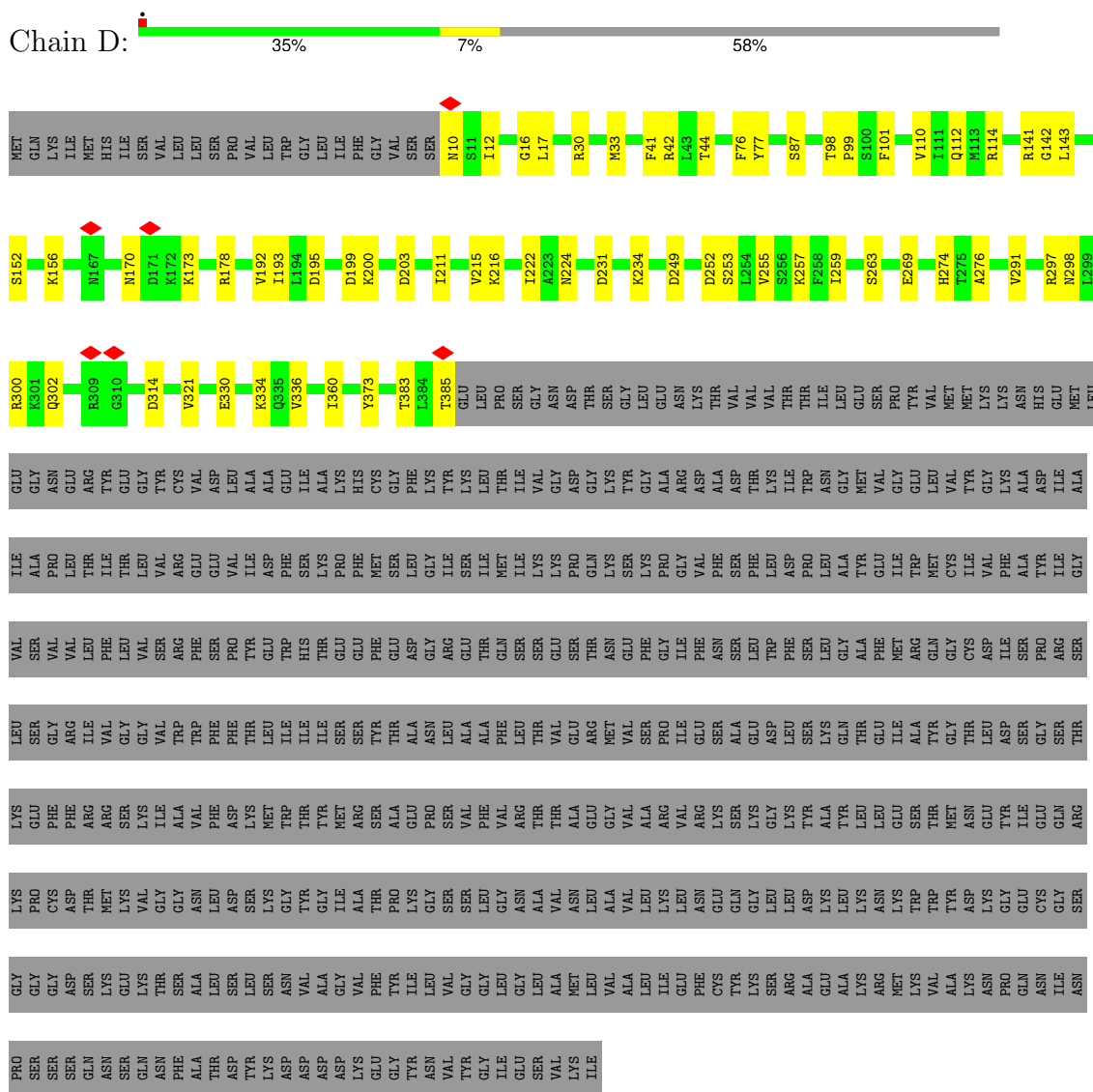


● Molecule 1: Glutamate receptor 2



ASP	LYS	GLY	ILE	ASP	GLY	ILE	MET	SER	GLU
LYS	GLU	VAL	ALA	ARG	ALA	ARG	ARG	SER	GLU
GLY	TYR	THR	THR	SER	THR	SER	SER	THR	PHE
TYR	TYR	ILE	PRO	ALA	LYS	GLY	ALA	ALA	THR
ASN	LEU	GLY	GLY	PRO	GLY	PRO	ASN	ASN	GLY
VAL	VAL	VAL	SER	SER	SER	SER	SER	LEU	ARG
TYR	GLY	GLY	SER	VAL	VAL	VAL	VAL	GLU	GLU
GLY	GLY	LEU	LEU	PHE	GLY	PHE	THR	ALA	THR
ILE	ILE	LEU	GLY	VAL	GLY	VAL	ARG	THR	GLN
GLU	GLY	GLY	ASN	ARG	ASN	ARG	THR	LEU	SER
SER	LEU	ALA	ALA	THR	THR	THR	THR	THR	SER
VAL	ALA	VAL	VAL	THR	VAL	VAL	THR	VAL	GLU
ILE	ILE	MET	ASN	ALA	ASN	ALA	GLY	GLU	SER
		VAL	ALA	GLY	ALA	VAL	VAL	MET	THR
		LEU	VAL	ARG	VAL	ALA	VAL	SER	GLU
		ILE	LYS	ARG	LEU	ARG	ALA	PRO	PHE
		GLU	GLY	VAL	LEU	VAL	ILE	ILE	GLY
		PHE	ASN	ARG	ASN	VAL	VAL	GLY	THR
		CYS	GLY	LYS	GLY	GLY	LYS	SER	ASN
		TYR	GLN	SER	GLN	GLY	SER	ALA	SER
		LYS	GLY	LYS	GLY	GLY	GLY	GLY	LEU
		SER	LEU	GLY	LEU	TYR	TYR	ASP	TRP
		ALA	LEU	LYS	LEU	TYR	TYR	GLY	THR
		ALA	ASN	LEU	LEU	LEU	ALA	GLN	GLY
		LYS	ASN	LEU	LEU	LEU	GLY	THR	ALA
		MET	LYS	GLY	GLY	GLY	ILE	GLU	PHE
		ARG	TRP	SER	LYS	SER	THR	ALA	MET
		VAL	TRP	THR	TRP	THR	THR	TYR	ARG
		ALA	TYR	MET	TYR	MET	GLN	GLY	GLN
		LYS	LYS	ASN	ASN	ASN	GLN	THR	CYS
		ASN	LYS	GLY	LYS	GLY	ARG	LEU	ASP
		PRO	GLY	TYR	ILE	TYR	LYS	SER	ILE
		GLN	GLU	ILE	GLY	GLY	GLY	PHE	SER
		ASN	ASN	GLY	CYS	CYS	PRO	GLY	GLY
		ILE	CYS	GLN	GLN	GLN	ARG	THR	ILE
		ASN	SER	ARG	THR	THR	ARG	ARG	VAL
		PRO	SER	GLY	PRO	PRO	LYS	SER	GLY
		SER	GLY	GLY	LYS	LYS	VAL	GLY	GLY
		SER	GLY	ASP	THR	THR	MET	ARG	THR
		GLN	SER	ASN	LYS	GLY	LYS	SER	VAL
		ASN	LYS	THR	GLY	THR	VAL	GLY	GLY
		SER	ASN	THR	THR	THR	GLY	ILE	VAL
		THR	LEU	LEU	ALA	ASN	ASN	TRP	TRP
		ASP	SER	ASP	LEU	LEU	ASP	PHE	PHE
		TYR	THR	LYS	SER	THR	LYS	THR	PHE
		LYS	ASN	LYS	ASN	GLY	LYS	MET	LEU
		ASP	ASN	GLY	ASN	GLY	GLY	TRP	ILE
		SER	ALA	TYR	VAL	VAL	TYR	THR	ILE
		ASP	ALA	GLY	ALA	GLY	GLY	THR	ILE
		SER	ALA	TYR	ASN	ASN	TYR	THR	ILE

- Molecule 1: Glutamate receptor 2



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



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



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



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



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 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, C2	Depositor
Number of particles used	122778	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 ( $e^-/\text{\AA}^2$ )	58.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0219	Depositor
Map size (Å)	383.76, 383.76, 383.76	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	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

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	0.27	0/2872	0.42	0/3915
1	B	0.27	0/2951	0.41	0/4012
1	C	0.27	0/2912	0.42	0/3969
1	D	0.27	0/2951	0.41	0/4012
All	All	0.27	0/11686	0.41	0/15908

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	2810	2366	2614	27	0
1	B	2889	2468	2768	37	0
1	C	2850	2442	2681	30	0
1	D	2889	2479	2768	40	0
2	E	28	12	25	0	0
2	G	28	12	25	1	0
2	I	28	12	25	0	0
2	K	28	12	25	1	0
3	F	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	39	0	34	1	0
3	J	39	0	34	1	0
3	L	39	0	34	1	0
All	All	11706	9803	11067	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:HIS:CD2	1:A:241:ASN:HB3	2.17	0.79
1:C:219:HIS:CD2	1:C:241:ASN:HB3	2.17	0.79
1:C:12:ILE:O	1:C:44:THR:OG1	2.08	0.70
1:C:105:GLY:O	1:C:352:LYS:NZ	2.25	0.69
1:A:105:GLY:O	1:A:352:LYS:NZ	2.25	0.69
1:C:151:ASP:OD1	1:C:152:SER:N	2.29	0.66
3:F:1:NAG:O3	3:F:2:NAG:O5	2.12	0.65
1:C:41:PHE:CZ	1:C:297:ARG:HB2	2.33	0.63
1:C:291:VAL:HG23	1:C:336:VAL:HG11	1.80	0.63
1:A:41:PHE:CZ	1:A:297:ARG:HB2	2.33	0.63
1:B:12:ILE:O	1:B:44:THR:N	2.32	0.62
1:A:249:ASP:O	1:A:255:VAL:HG11	2.00	0.62
1:C:249:ASP:O	1:C:255:VAL:HG11	2.00	0.62
1:A:291:VAL:HG23	1:A:336:VAL:HG11	1.80	0.62
1:D:291:VAL:HG23	1:D:336:VAL:HG11	1.81	0.62
1:C:30:ARG:NH2	1:C:269:GLU:O	2.33	0.62
1:D:12:ILE:O	1:D:44:THR:N	2.32	0.61
1:B:170:ASN:O	1:B:173:LYS:HG2	2.01	0.61
1:A:263:SER:O	1:A:274:HIS:ND1	2.34	0.61
1:B:291:VAL:HG23	1:B:336:VAL:HG11	1.81	0.61
1:C:263:SER:O	1:C:274:HIS:ND1	2.34	0.61
1:A:30:ARG:NH2	1:A:269:GLU:O	2.33	0.60
1:D:170:ASN:O	1:D:173:LYS:HG2	2.01	0.60
1:C:372:GLY:HA2	1:C:383:THR:HG22	1.84	0.60
1:B:77:TYR:HE1	1:B:98:THR:HG21	1.67	0.60
1:D:77:TYR:HE1	1:D:98:THR:HG21	1.67	0.59
3:J:1:NAG:O3	3:J:2:NAG:O5	2.12	0.59
1:A:372:GLY:HA2	1:A:383:THR:HG22	1.84	0.58
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.37	0.57
1:A:128:TYR:OH	1:A:362:GLU:OE2	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASN:O	1:B:302:GLN:HG3	2.06	0.55
1:D:298:ASN:O	1:D:302:GLN:HG3	2.06	0.55
1:C:128:TYR:OH	1:C:362:GLU:OE2	2.21	0.55
1:D:77:TYR:OH	1:D:101:PHE:O	2.10	0.55
1:B:77:TYR:OH	1:B:101:PHE:O	2.10	0.55
1:C:252:ASP:HB3	1:C:255:VAL:HG12	1.89	0.55
1:B:141:ARG:NH2	1:B:195:ASP:OD1	2.37	0.54
1:D:99:PRO:O	1:D:114:ARG:HB2	2.08	0.54
1:B:99:PRO:O	1:B:114:ARG:HB2	2.08	0.54
1:C:99:PRO:O	1:C:114:ARG:HB2	2.08	0.54
1:A:252:ASP:HB3	1:A:255:VAL:HG12	1.89	0.54
1:C:199:ASP:OD1	1:C:200:LYS:N	2.40	0.54
1:B:252:ASP:HB3	1:B:255:VAL:HG12	1.90	0.53
1:A:99:PRO:O	1:A:114:ARG:HB2	2.08	0.53
1:B:142:GLY:O	1:B:143:LEU:HD23	2.09	0.52
1:D:252:ASP:HB3	1:D:255:VAL:HG12	1.90	0.52
1:A:183:ASP:HA	1:A:186:LEU:HD13	1.92	0.52
1:D:142:GLY:O	1:D:143:LEU:HD23	2.09	0.52
1:A:185:GLU:OE2	1:A:213:LYS:NZ	2.43	0.52
1:C:54:ASN:OD1	1:D:87:SER:OG	2.28	0.52
1:D:199:ASP:OD1	1:D:200:LYS:N	2.44	0.51
1:C:183:ASP:HA	1:C:186:LEU:HD13	1.92	0.51
2:K:2:NAG:O7	2:K:2:NAG:O3	2.28	0.51
1:C:185:GLU:OE2	1:C:213:LYS:NZ	2.43	0.50
1:B:199:ASP:OD1	1:B:200:LYS:N	2.44	0.50
1:B:178:ARG:HG2	1:B:211:ILE:HD11	1.94	0.50
1:A:79:LYS:HG2	1:A:139:SER:O	2.13	0.49
1:D:178:ARG:HG2	1:D:211:ILE:HD11	1.94	0.49
1:D:16:GLY:C	1:D:17:LEU:HD12	2.34	0.48
1:D:383:THR:HG22	1:D:385:THR:CG2	2.44	0.48
1:B:16:GLY:C	1:B:17:LEU:HD12	2.34	0.48
1:D:330:GLU:OE2	1:D:334:LYS:NZ	2.32	0.48
1:B:222:ILE:HG22	1:B:224:ASN:OD1	2.14	0.48
2:G:2:NAG:O7	2:G:2:NAG:O3	2.28	0.48
1:B:33:MET:HE3	1:B:42:ARG:HH22	1.79	0.48
1:C:79:LYS:HG2	1:C:139:SER:O	2.13	0.48
1:D:33:MET:HE3	1:D:42:ARG:HH22	1.79	0.48
1:B:383:THR:HG22	1:B:385:THR:CG2	2.44	0.47
1:A:54:ASN:OD1	1:B:87:SER:OG	2.32	0.47
1:A:77:TYR:CE1	1:A:98:THR:HG21	2.49	0.47
1:C:344:ASN:O	1:C:353:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ILE:HG22	1:D:224:ASN:OD1	2.14	0.47
1:C:77:TYR:CE1	1:C:98:THR:HG21	2.49	0.47
1:C:372:GLY:CA	1:C:383:THR:HG22	2.46	0.46
1:D:142:GLY:C	1:D:143:LEU:HD23	2.35	0.46
1:D:321:VAL:HG23	1:D:321:VAL:O	2.16	0.46
1:A:372:GLY:CA	1:A:383:THR:HG22	2.46	0.46
1:B:142:GLY:C	1:B:143:LEU:HD23	2.36	0.46
1:B:259:ILE:HD12	1:B:276:ALA:O	2.16	0.46
1:B:383:THR:HG22	1:B:385:THR:HG22	1.99	0.45
1:D:383:THR:HG22	1:D:385:THR:HG22	1.99	0.45
1:B:41:PHE:HE2	1:B:297:ARG:HB2	1.81	0.45
1:A:382:VAL:O	1:A:382:VAL:HG23	2.16	0.45
1:C:382:VAL:O	1:C:382:VAL:HG23	2.16	0.45
1:B:321:VAL:O	1:B:321:VAL:HG23	2.16	0.45
1:D:41:PHE:HE2	1:D:297:ARG:HB2	1.81	0.45
1:D:259:ILE:HD12	1:D:276:ALA:O	2.16	0.45
1:B:314:ASP:N	1:B:314:ASP:OD1	2.49	0.45
1:D:253:SER:O	1:D:257:LYS:HG3	2.17	0.45
1:B:330:GLU:OE2	1:B:334:LYS:NZ	2.32	0.45
1:D:314:ASP:OD1	1:D:314:ASP:N	2.49	0.45
1:B:253:SER:O	1:B:257:LYS:HG3	2.17	0.44
1:B:173:LYS:HD3	1:B:203:ASP:OD2	2.18	0.44
1:B:249:ASP:O	1:B:255:VAL:HG11	2.18	0.44
1:D:173:LYS:HD3	1:D:203:ASP:OD2	2.18	0.43
1:D:231:ASP:OD2	1:D:234:LYS:NZ	2.43	0.43
1:C:247:ILE:HG23	1:C:248:VAL:HG13	2.01	0.43
1:D:360:ILE:HD12	1:D:373:TYR:HA	2.01	0.43
1:B:360:ILE:HD12	1:B:373:TYR:HA	2.01	0.43
1:C:10:ASN:ND2	1:C:40:GLU:O	2.44	0.43
1:D:263:SER:O	1:D:274:HIS:ND1	2.52	0.43
1:D:249:ASP:O	1:D:255:VAL:HG11	2.18	0.42
1:A:247:ILE:HG23	1:A:248:VAL:HG13	2.01	0.42
1:B:263:SER:O	1:B:274:HIS:ND1	2.52	0.42
1:A:344:ASN:O	1:A:353:ARG:NH2	2.47	0.42
1:A:371:ILE:HA	1:A:384:LEU:HB2	2.01	0.42
1:D:170:ASN:HA	1:D:173:LYS:HE3	2.01	0.42
1:B:170:ASN:HA	1:B:173:LYS:HE3	2.01	0.42
1:A:131:ASP:OD1	1:A:131:ASP:N	2.53	0.42
1:D:152:SER:O	1:D:156:LYS:HG2	2.20	0.42
1:B:77:TYR:CE1	1:B:98:THR:HG21	2.51	0.42
1:C:131:ASP:N	1:C:131:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:VAL:HG12	1:D:193:ILE:N	2.35	0.42
1:A:23:ASP:OD1	1:A:24:GLN:N	2.54	0.41
1:C:371:ILE:HA	1:C:384:LEU:HB2	2.01	0.41
1:A:41:PHE:HZ	1:A:297:ARG:HB2	1.84	0.41
1:B:152:SER:O	1:B:156:LYS:HG2	2.20	0.41
1:D:10:ASN:HD21	1:D:300:ARG:HH21	1.68	0.41
1:D:385:THR:OG1	1:D:385:THR:O	2.38	0.41
1:D:110:VAL:HG12	1:D:112:GLN:OE1	2.20	0.41
1:C:383:THR:HG23	1:C:384:LEU:N	2.35	0.41
3:L:1:NAG:H61	3:L:2:NAG:N2	2.35	0.41
3:H:1:NAG:H61	3:H:2:NAG:N2	2.35	0.41
1:D:30:ARG:NH1	1:D:269:GLU:O	2.54	0.41
1:D:76:PHE:N	1:D:76:PHE:CD1	2.89	0.41
1:D:77:TYR:CE1	1:D:98:THR:HG21	2.50	0.41
1:A:215:VAL:HG22	1:A:216:LYS:N	2.36	0.41
1:C:77:TYR:HE1	1:C:98:THR:HG21	1.86	0.41
1:B:110:VAL:HG12	1:B:112:GLN:OE1	2.20	0.40
1:B:192:VAL:HG12	1:B:193:ILE:N	2.35	0.40
1:C:215:VAL:HG22	1:C:216:LYS:N	2.36	0.40
1:A:10:ASN:ND2	1:A:40:GLU:O	2.44	0.40
1:A:383:THR:HG23	1:A:384:LEU:N	2.35	0.40
1:B:385:THR:OG1	1:B:385:THR:O	2.38	0.40
1:B:10:ASN:HD21	1:B:300:ARG:HE	1.70	0.40
1:B:10:ASN:HD21	1:B:300:ARG:HH21	1.69	0.40
1:D:215:VAL:HG22	1:D:216:LYS:N	2.37	0.40
1:C:23:ASP:OD1	1:C:24:GLN:N	2.54	0.40

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	374/889 (42%)	367 (98%)	7 (2%)	0	100	100
1	B	374/889 (42%)	356 (95%)	18 (5%)	0	100	100
1	C	374/889 (42%)	367 (98%)	7 (2%)	0	100	100
1	D	374/889 (42%)	356 (95%)	18 (5%)	0	100	100
All	All	1496/3556 (42%)	1446 (97%)	50 (3%)	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	275/761 (36%)	274 (100%)	1 (0%)	89	93
1	B	299/761 (39%)	299 (100%)	0	100	100
1	C	291/761 (38%)	290 (100%)	1 (0%)	91	94
1	D	299/761 (39%)	299 (100%)	0	100	100
All	All	1164/3044 (38%)	1162 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	C	79	LYS

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

Mol	Chain	Res	Type
1	A	60	ASN
1	A	290	GLN
1	B	337	GLN
1	C	10	ASN
1	C	60	ASN

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Mol	Chain	Res	Type
1	C	290	GLN
1	D	337	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 ⓘ

20 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	$\# Z  > 2$
2	NAG	E	1	1,2	14,14,15	0.22	0	17,19,21	1.02	1 (5%)
2	NAG	E	2	2	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	F	1	1,3	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.43	0
3	BMA	F	3	3	11,11,12	0.59	0	15,15,17	0.73	0
2	NAG	G	1	1,2	14,14,15	0.56	0	17,19,21	0.37	0
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	H	1	1,3	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	H	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	BMA	H	3	3	11,11,12	0.56	0	15,15,17	0.73	0
2	NAG	I	1	1,2	14,14,15	0.21	0	17,19,21	1.02	1 (5%)
2	NAG	I	2	2	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	J	1	1,3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	BMA	J	3	3	11,11,12	0.59	0	15,15,17	0.73	0
2	NAG	K	1	1,2	14,14,15	0.56	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	K	2	2	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	L	1	1,3	14,14,15	0.19	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	BMA	L	3	3	11,11,12	0.57	0	15,15,17	0.74	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	1/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C2-N2-C7	3.81	128.01	122.90
2	I	1	NAG	C2-N2-C7	3.78	127.97	122.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
3	H	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7

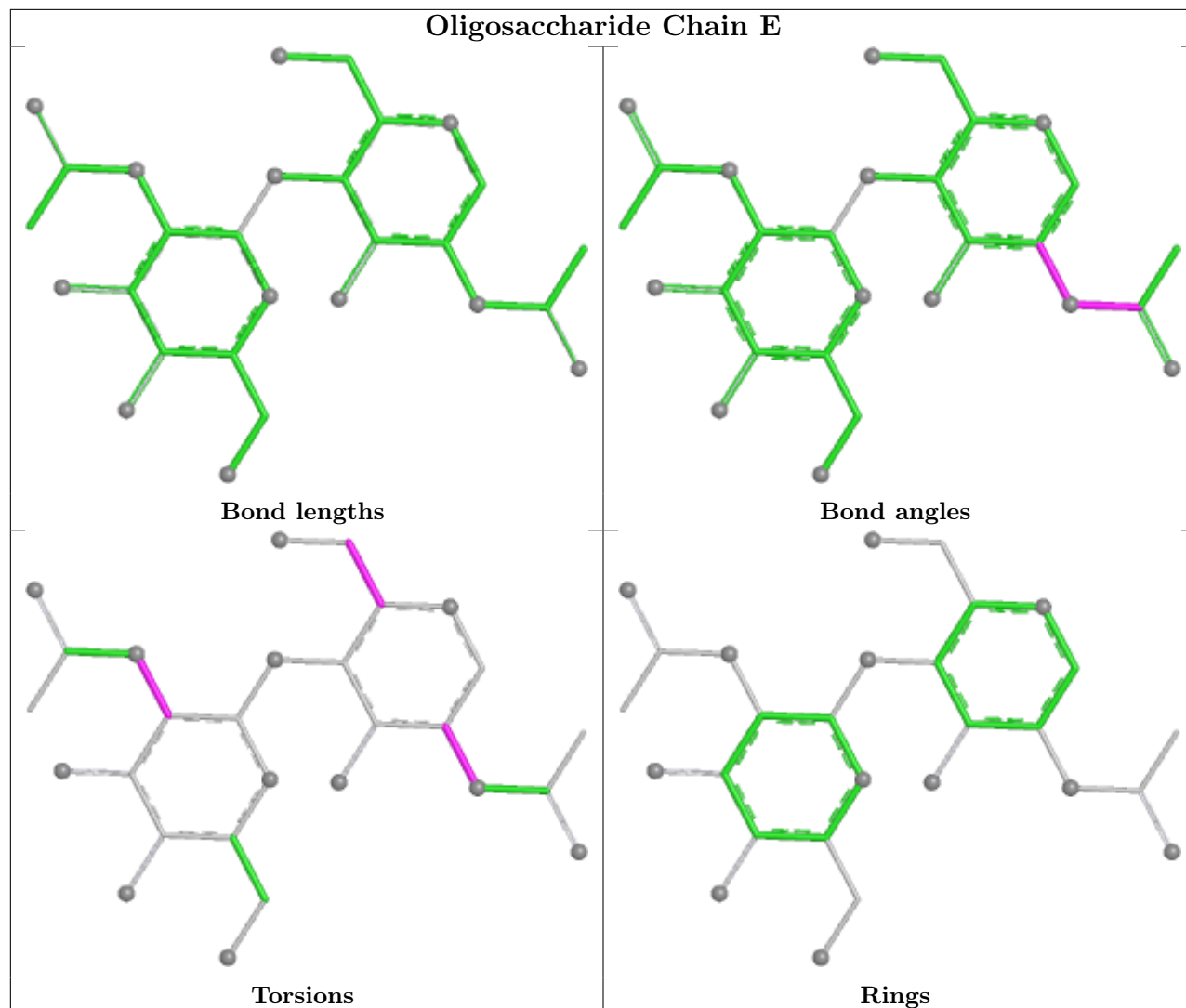
There are no ring outliers.

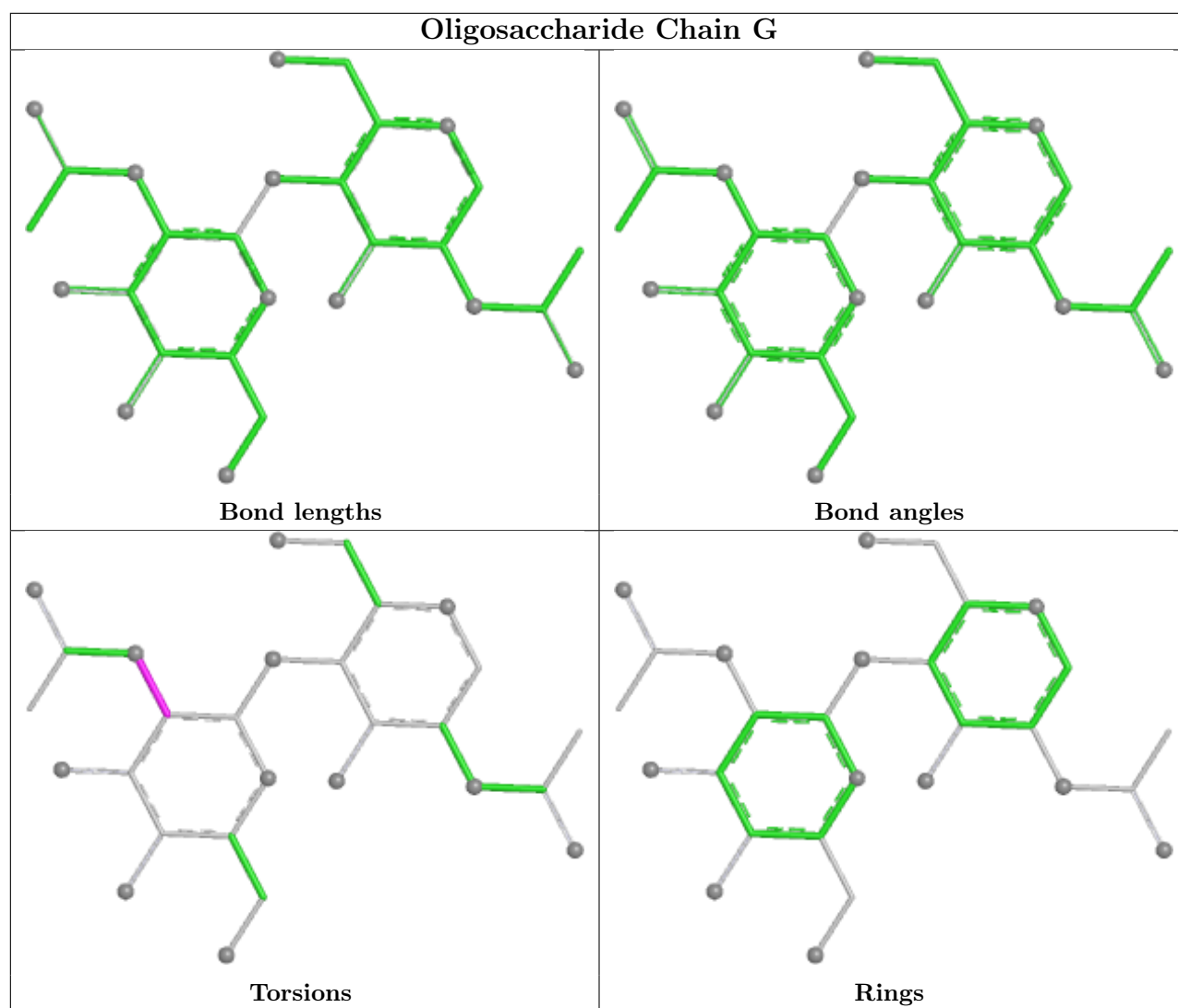
10 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	F	1	NAG	1	0
3	L	1	NAG	1	0
3	L	2	NAG	1	0
3	F	2	NAG	1	0
2	K	2	NAG	1	0
3	J	1	NAG	1	0
3	J	2	NAG	1	0
2	G	2	NAG	1	0
3	H	2	NAG	1	0

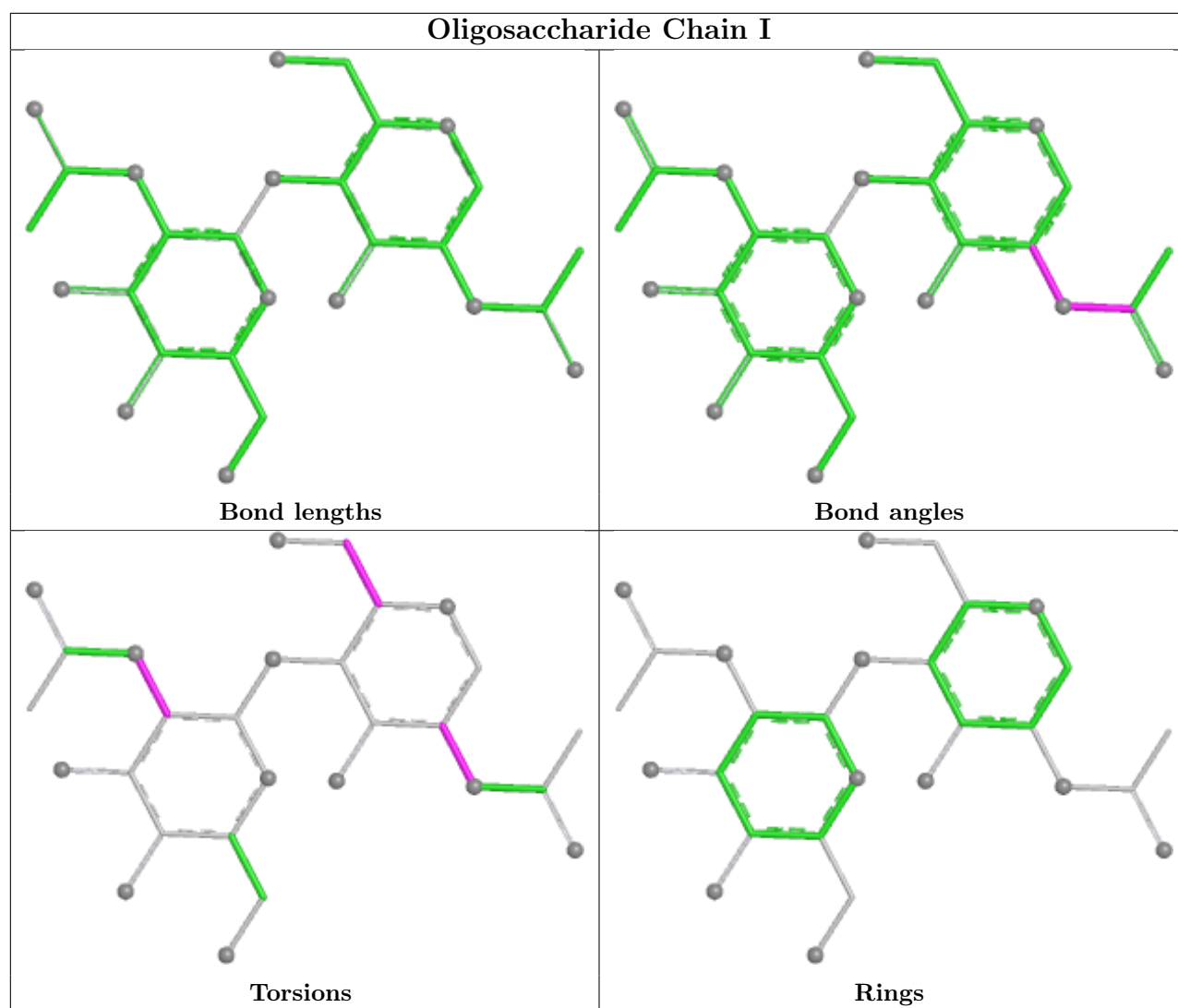
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

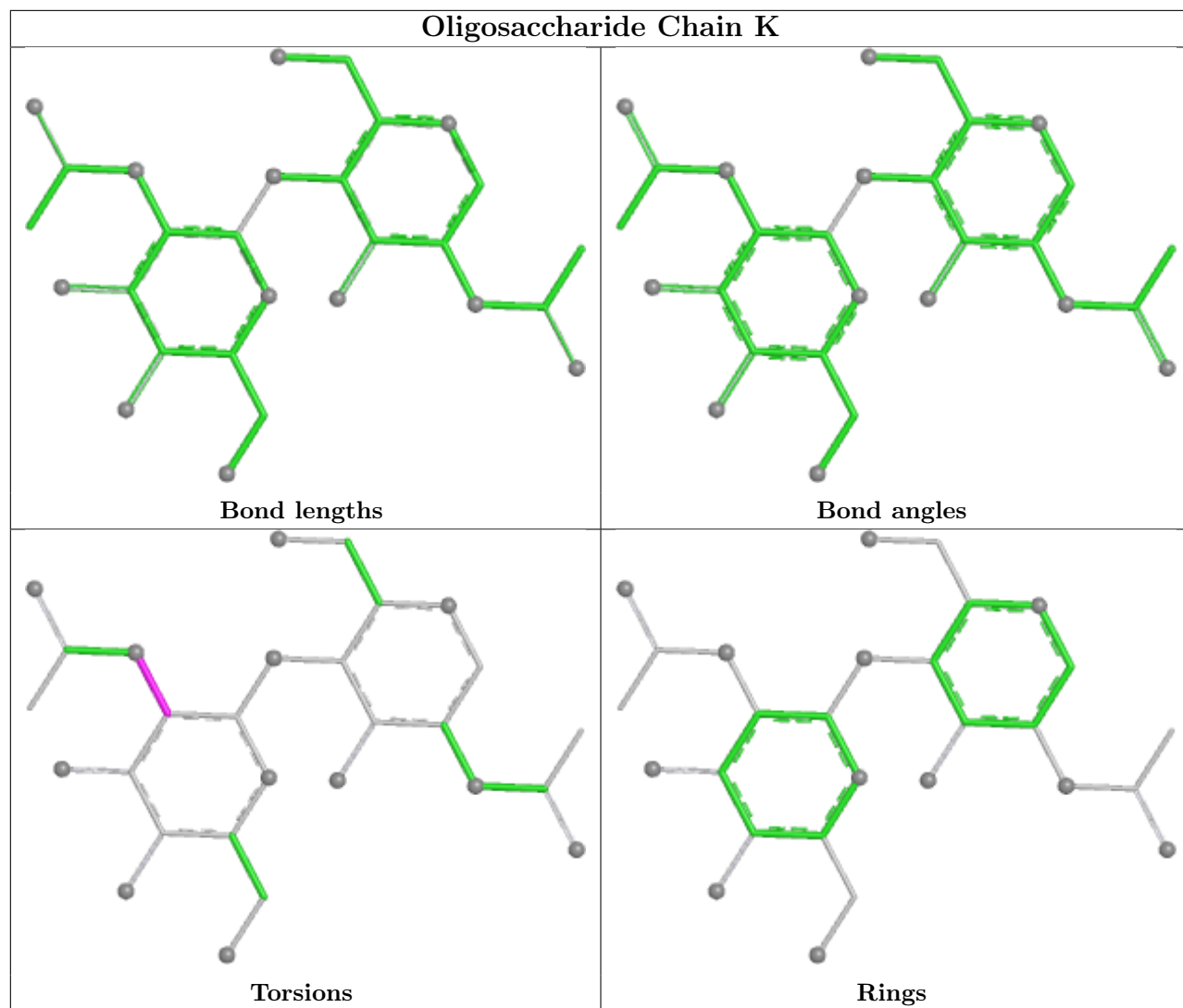
bond angles, torsion angles, and ring geometry for oligosaccharide.

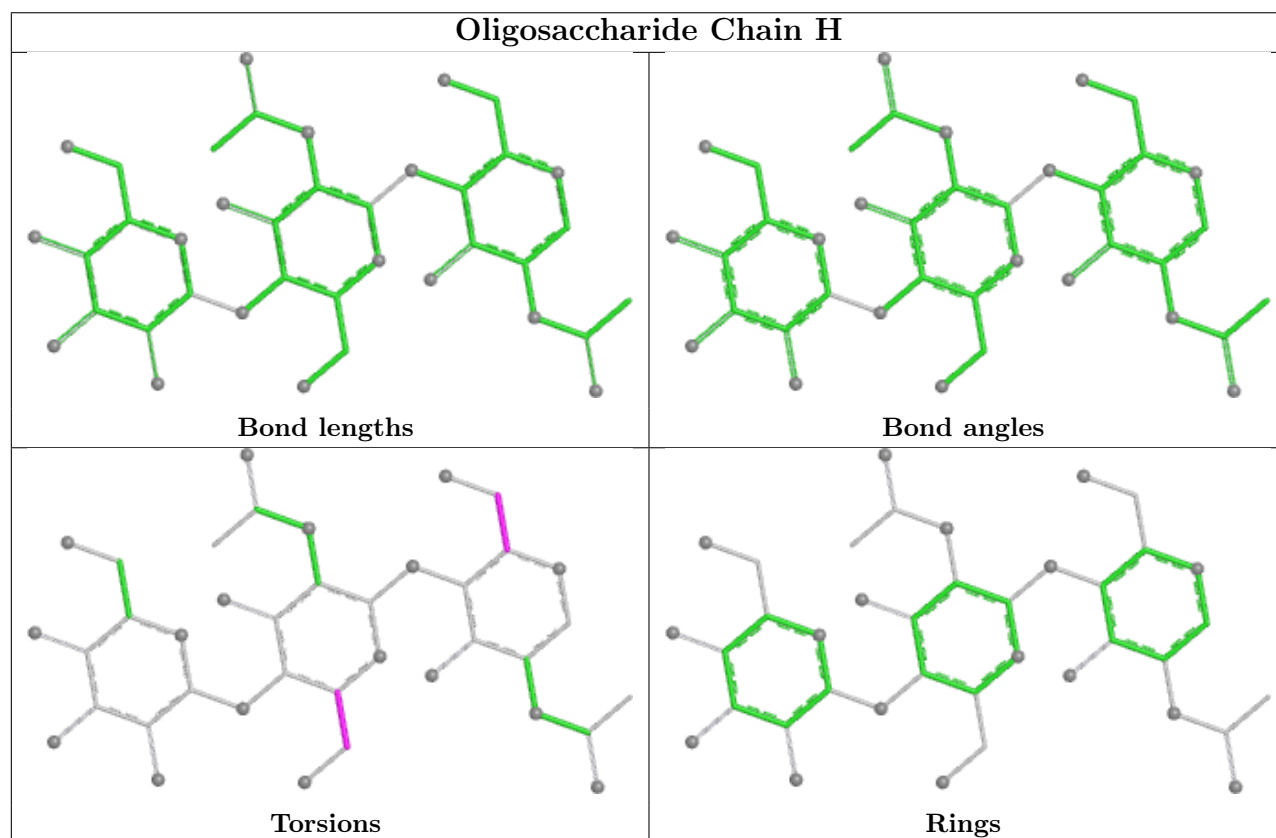
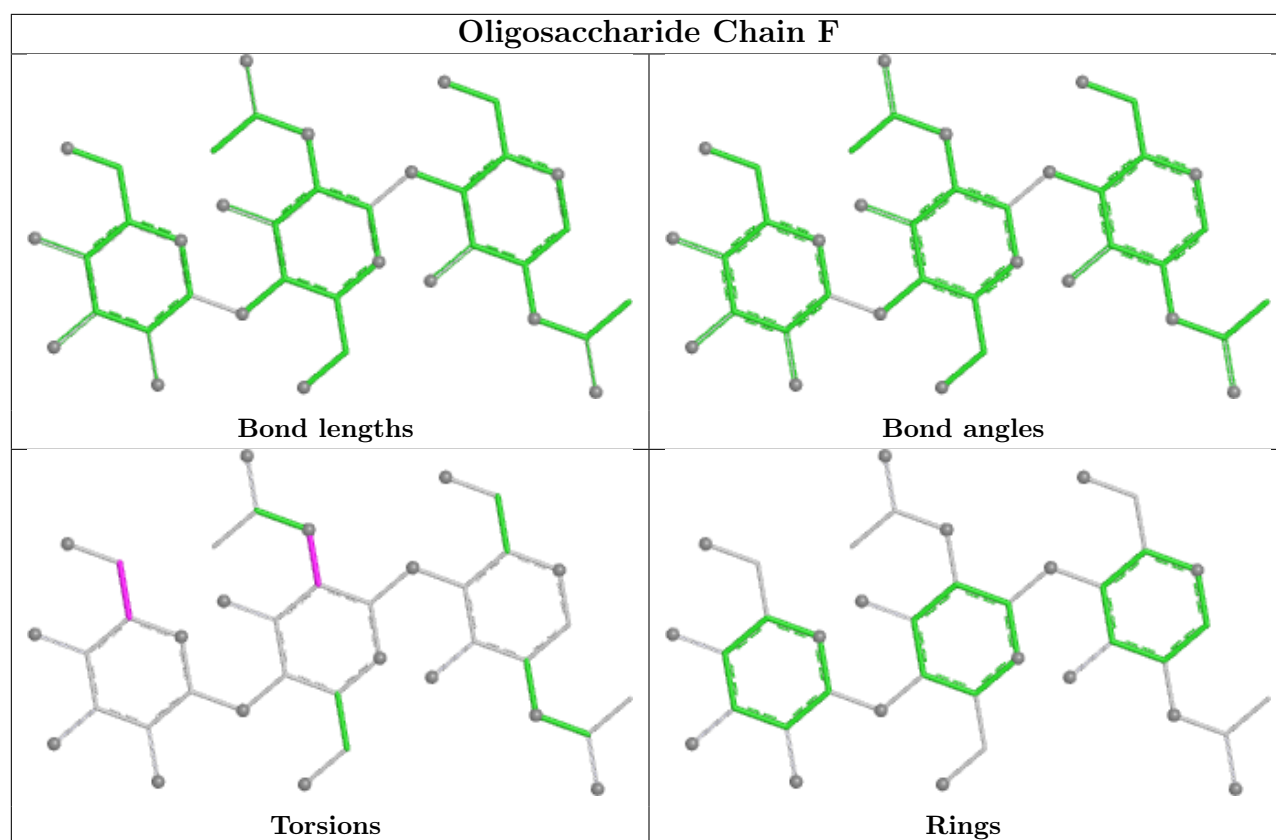


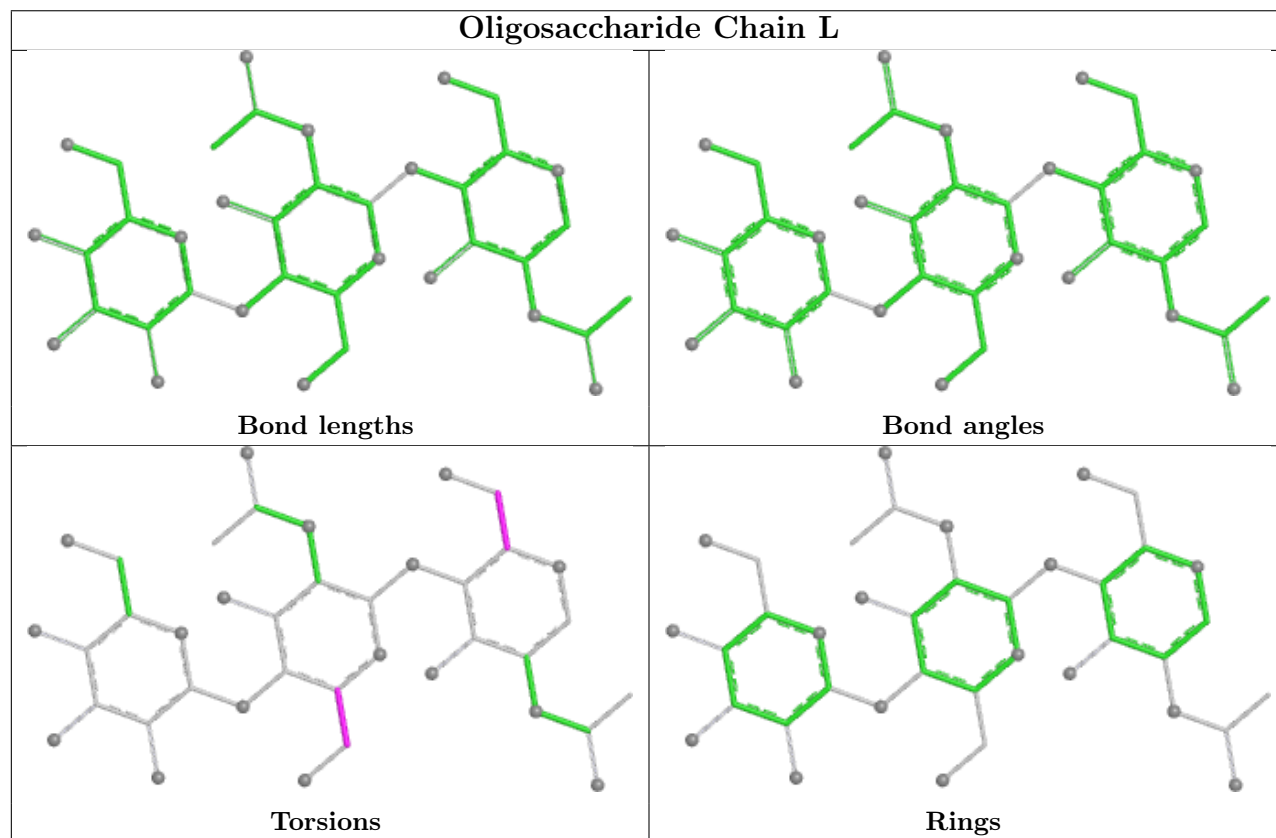
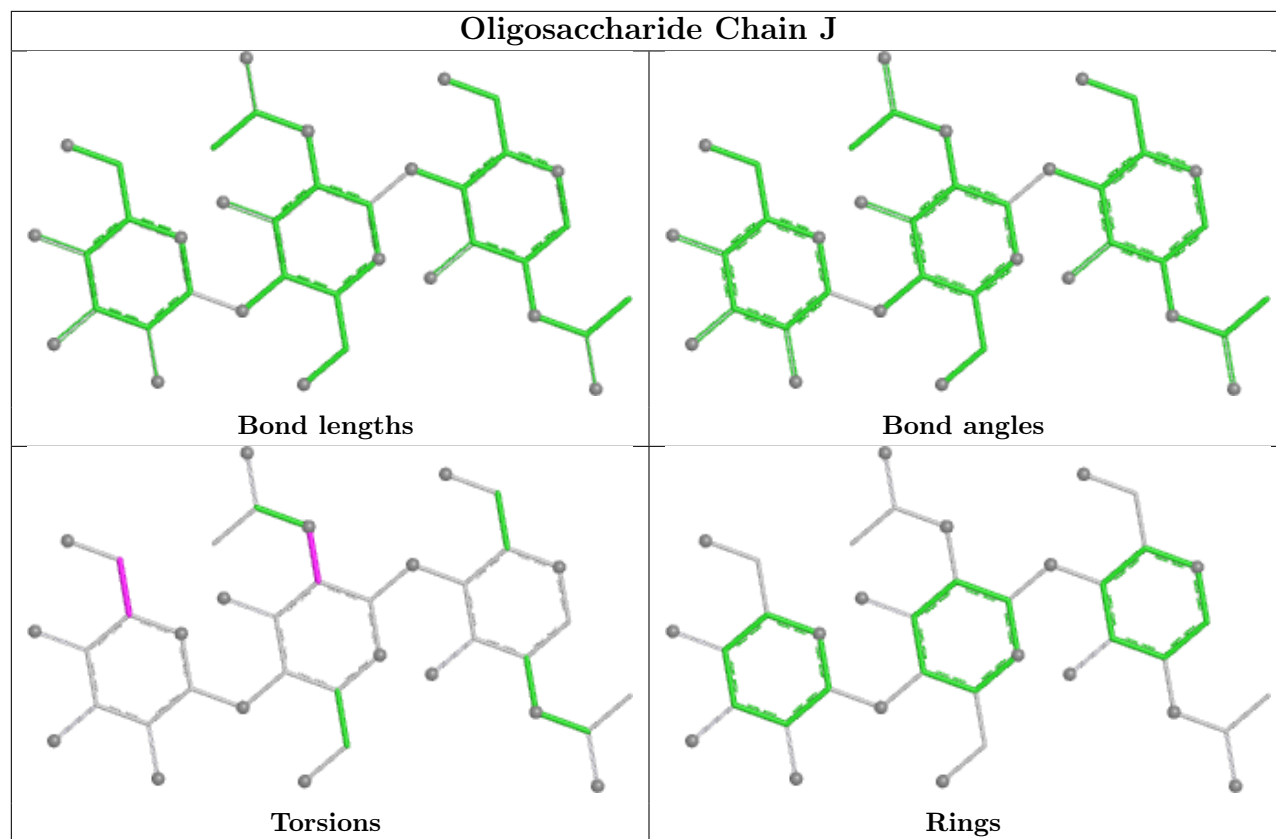












## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

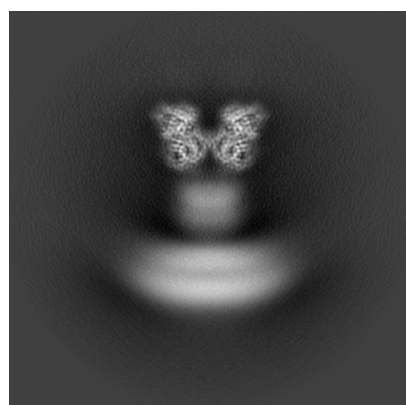
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20654. These allow visual inspection of the internal detail of the map and identification of artifacts.

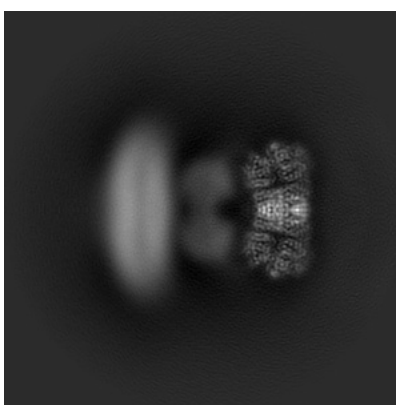
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

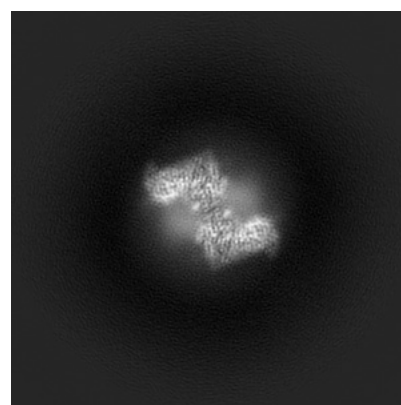
#### 6.1.1 Primary map



X



Y

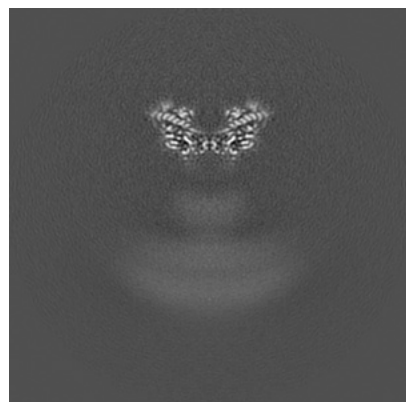


Z

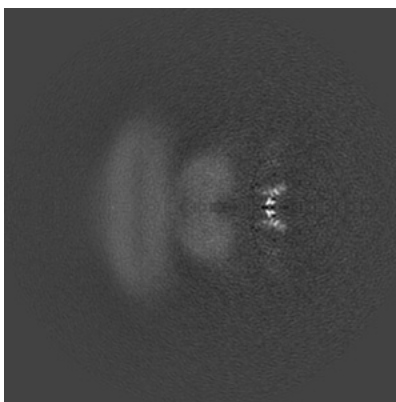
The images above show the map projected in three orthogonal directions.

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

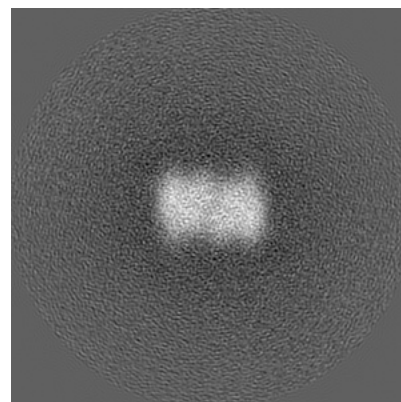
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

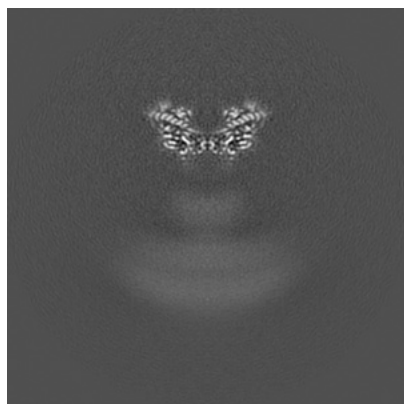


Z Index: 180

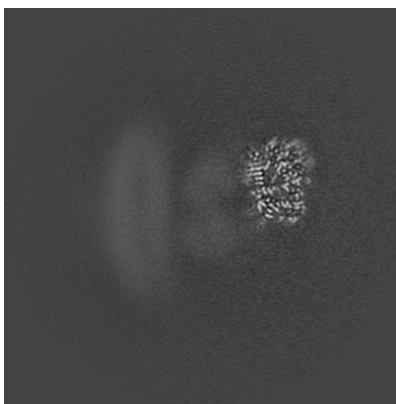
The images above show central slices of the map in three orthogonal directions.

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

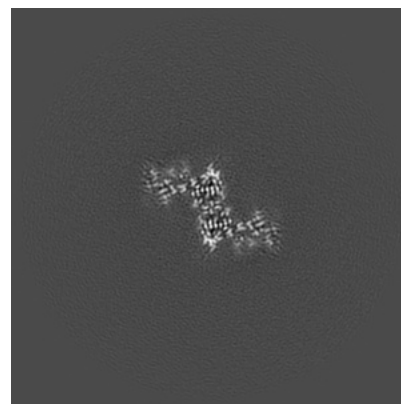
### 6.3.1 Primary map



X Index: 180



Y Index: 157



Z Index: 238

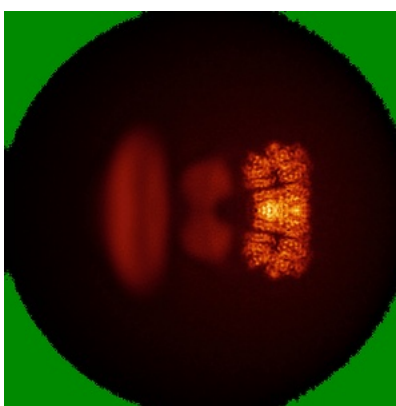
The images above show the largest variance slices of the map in three orthogonal directions.

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

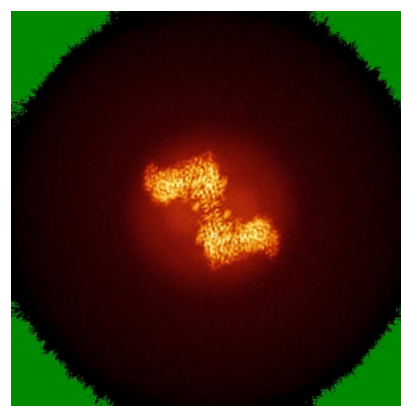
### 6.4.1 Primary map



X



Y

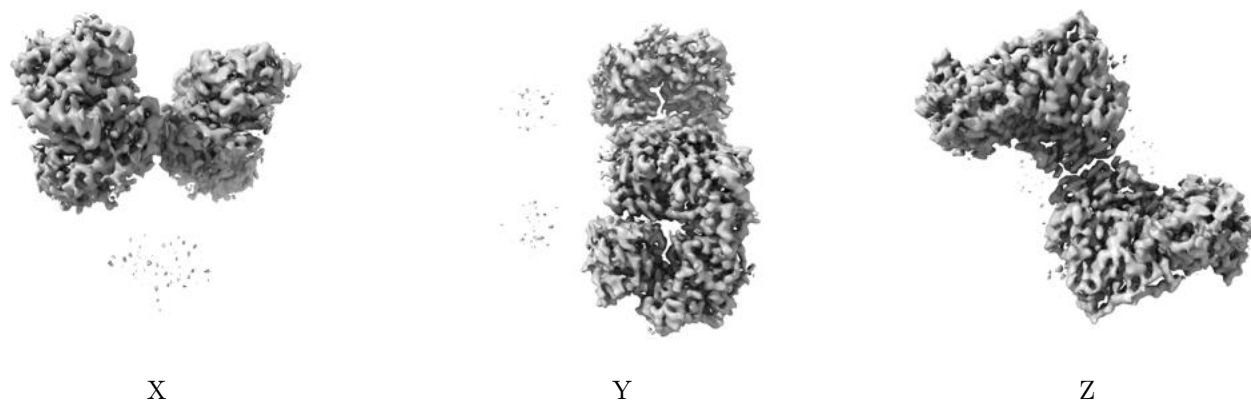


Z

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 0.0219. 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](#)

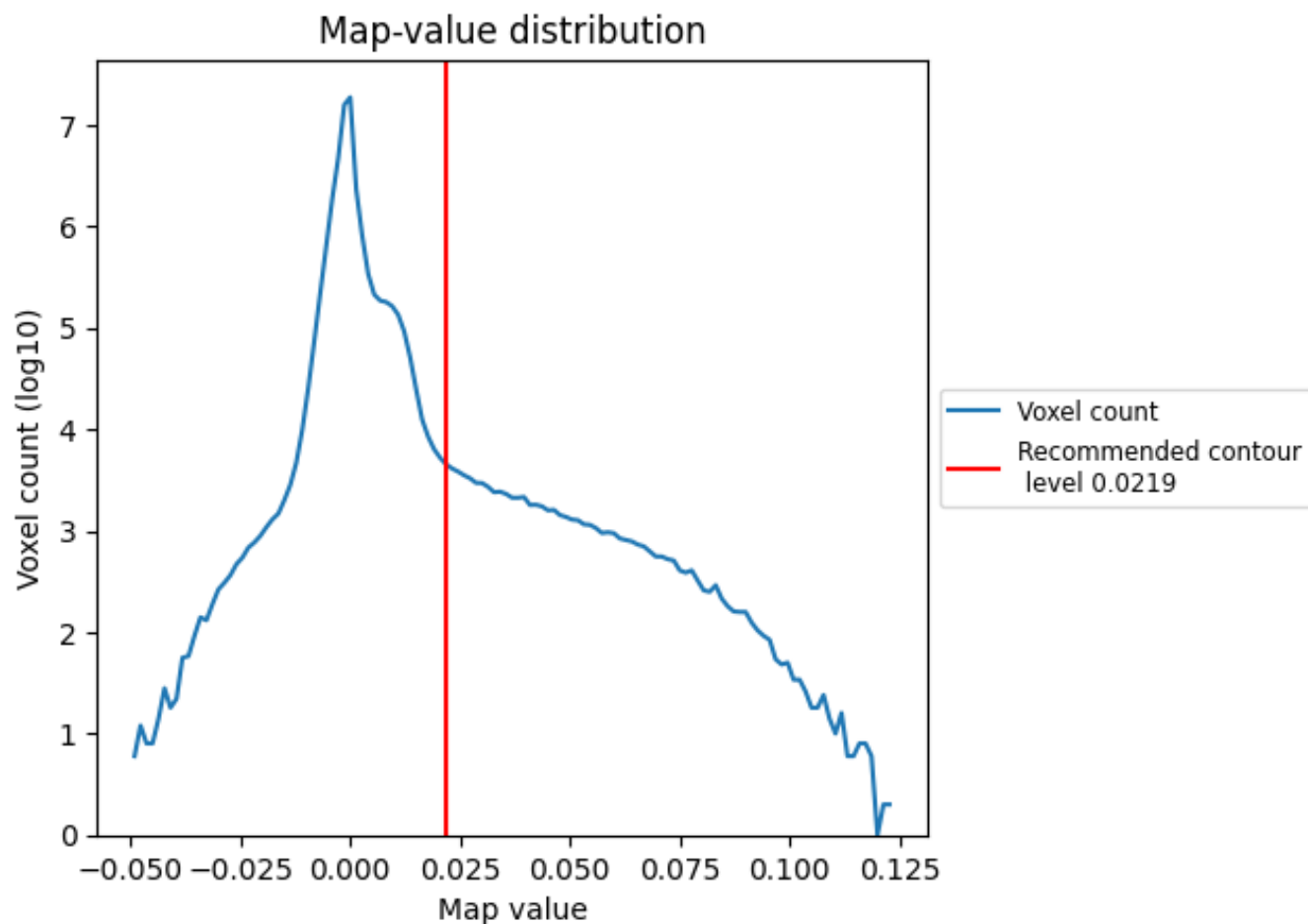
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

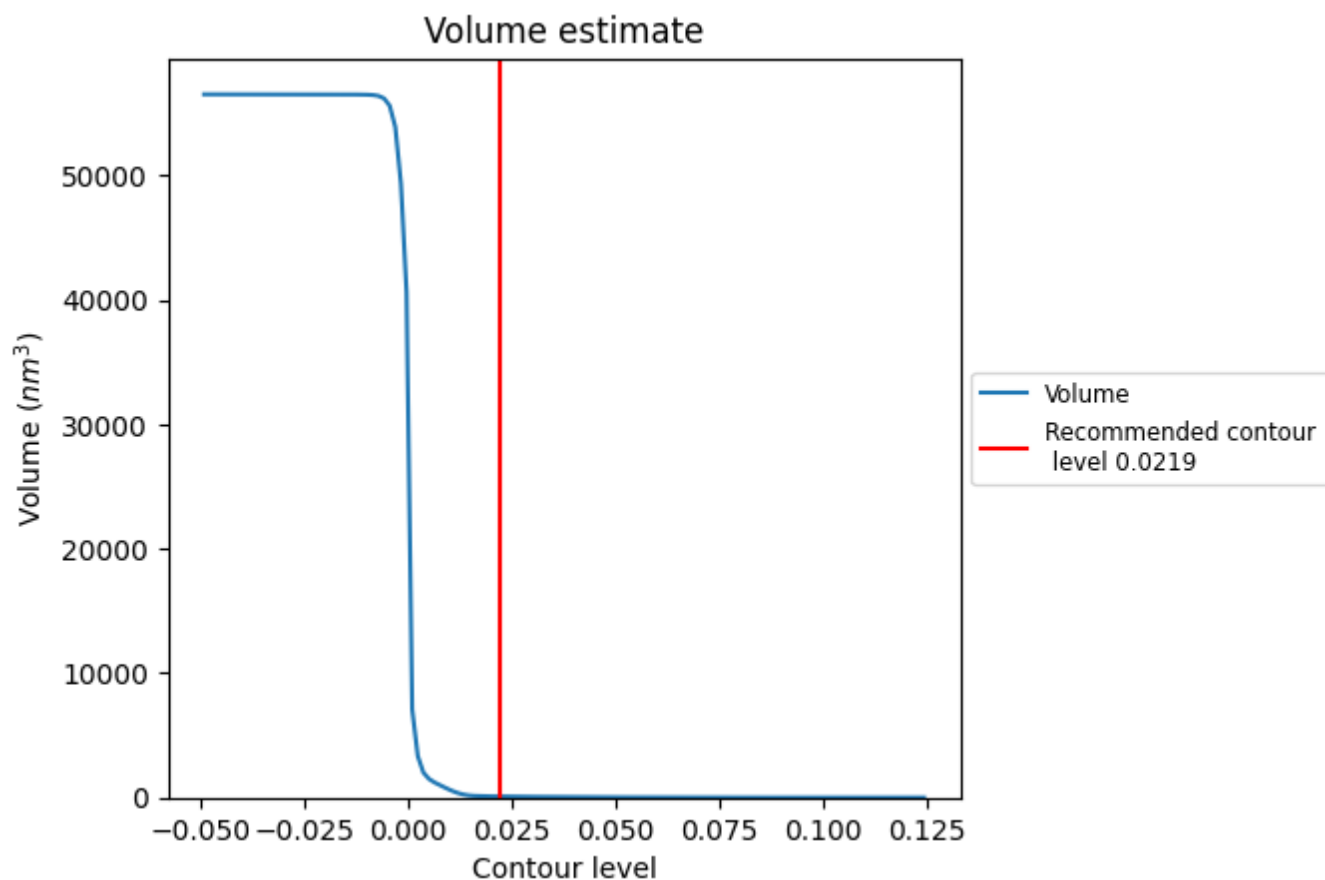
This section contains the results of statistical analysis of the map.

### 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.

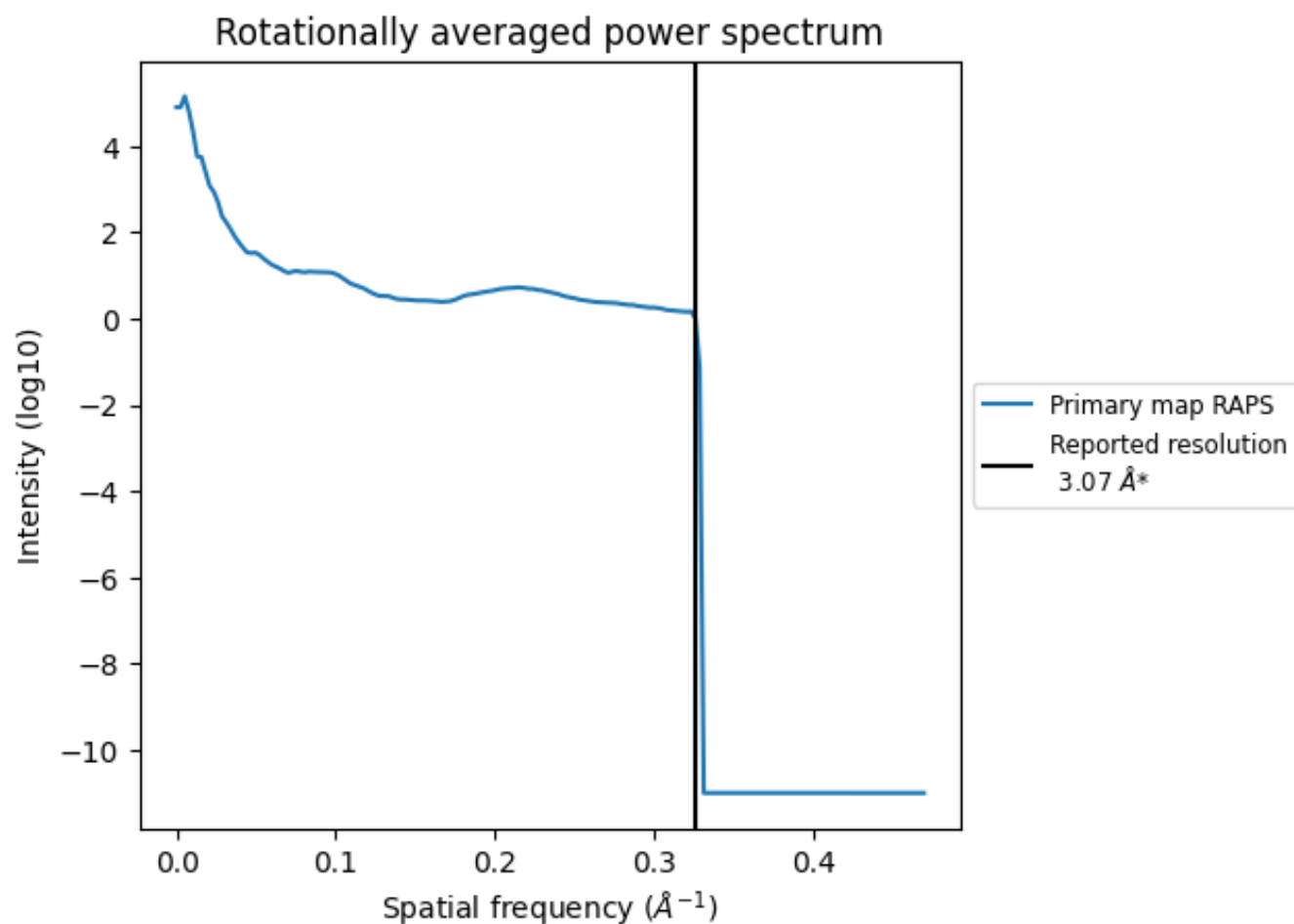
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm<sup>3</sup>; this corresponds to an approximate mass of 79 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 ⓘ

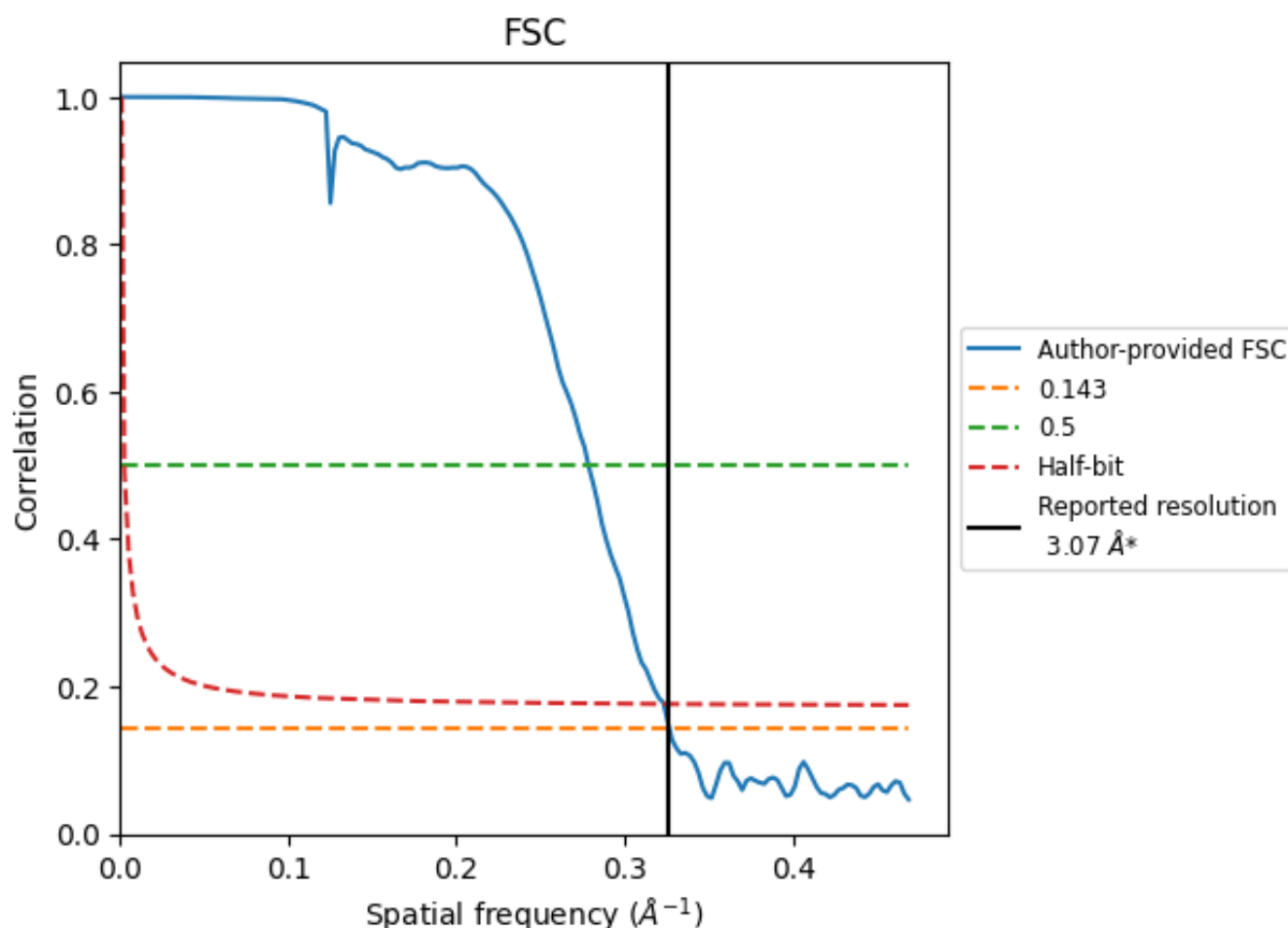


\*Reported resolution corresponds to spatial frequency of 0.326 Å<sup>-1</sup>

## 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 0.326 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

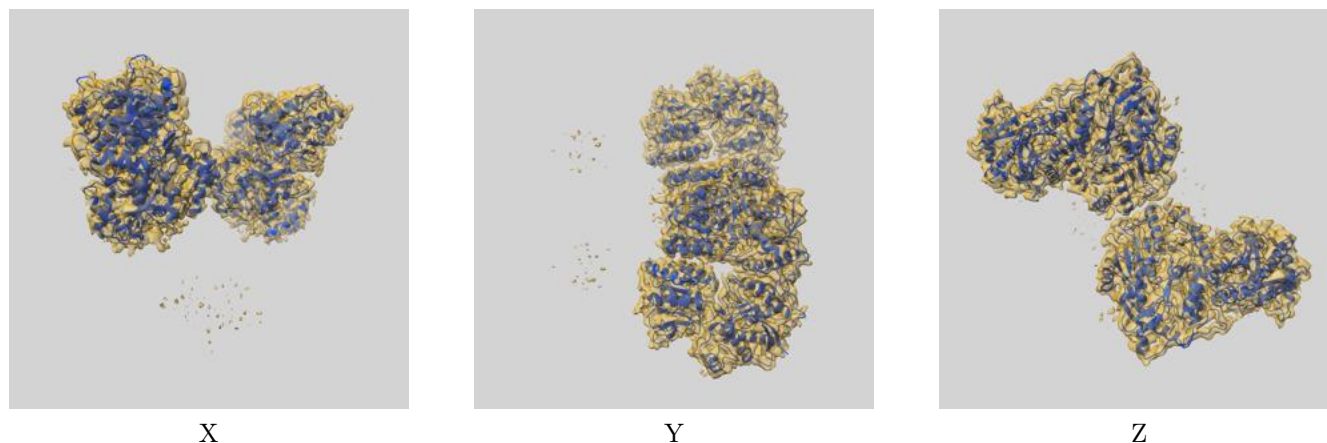
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.06	3.59	3.09
Unmasked-calculated*	-	-	-

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

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

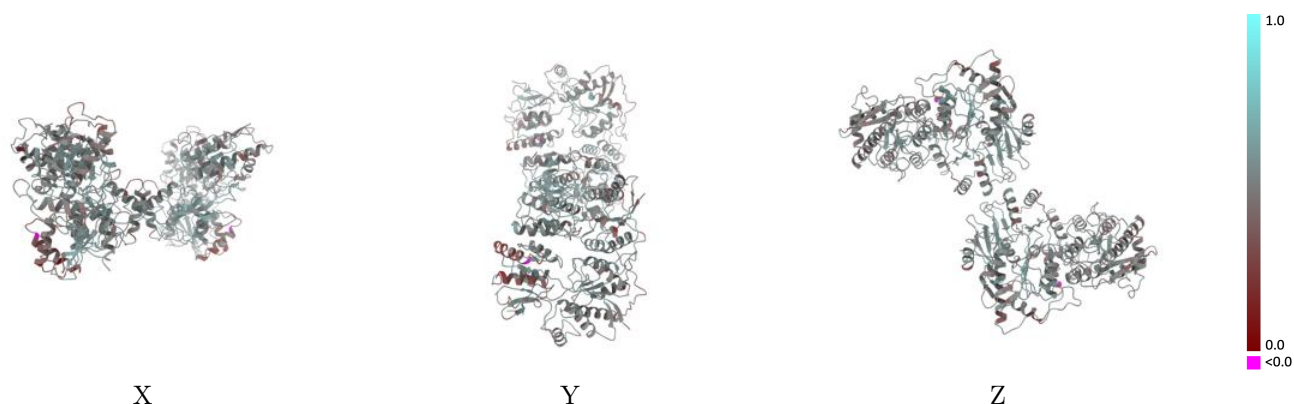
This section contains information regarding the fit between EMDB map EMD-20654 and PDB model 6U5S. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



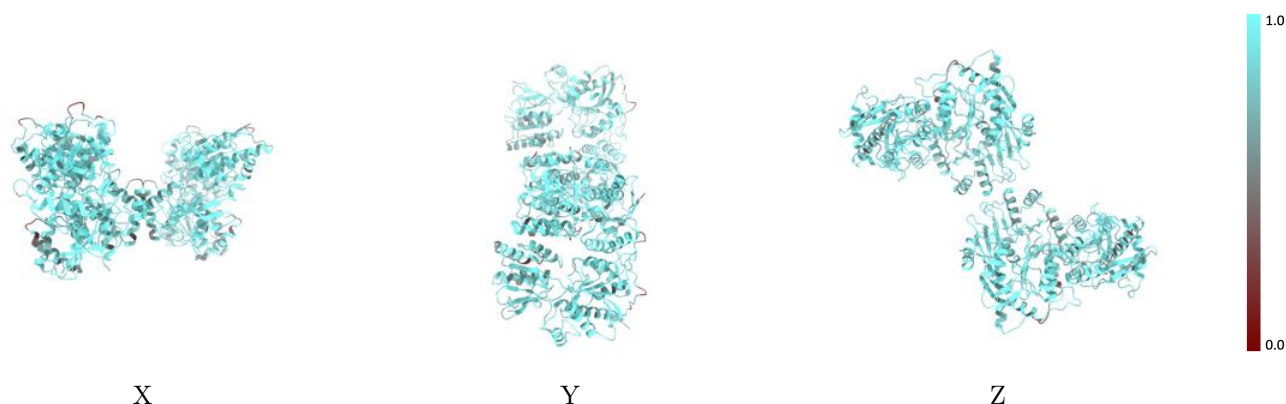
The images above show the 3D surface view of the map at the recommended contour level 0.0219 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



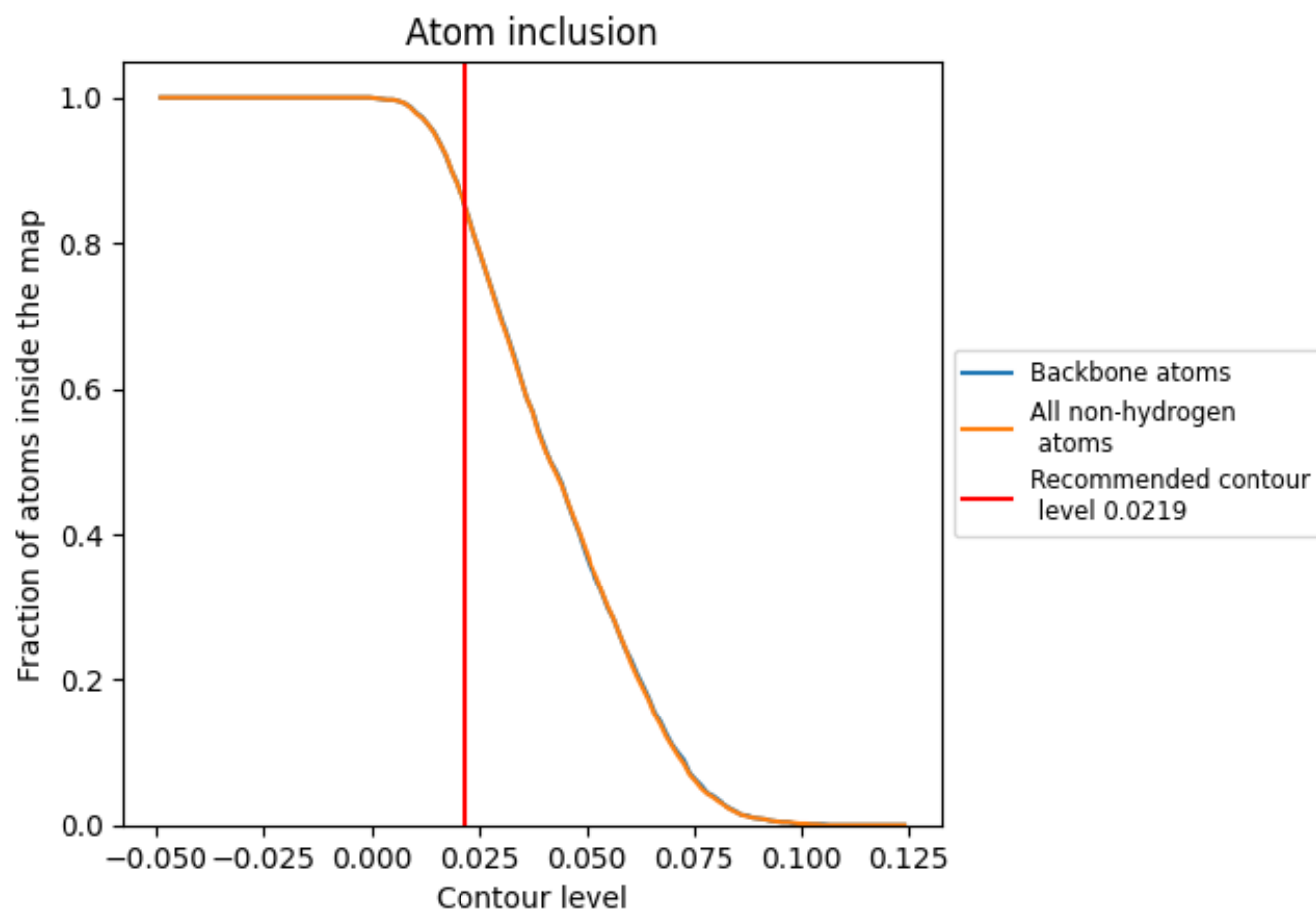
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0219).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.0219) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8500	<div></div> 0.4990
A	<div></div> 0.8540	<div></div> 0.4850
B	<div></div> 0.8810	<div></div> 0.5170
C	<div></div> 0.8390	<div></div> 0.4810
D	<div></div> 0.8810	<div></div> 0.5170
E	<div></div> 0.4640	<div></div> 0.4130
F	<div></div> 0.3590	<div></div> 0.3900
G	<div></div> 0.3210	<div></div> 0.4630
H	<div></div> 0.4870	<div></div> 0.5240
I	<div></div> 0.5710	<div></div> 0.4270
J	<div></div> 0.3590	<div></div> 0.3940
K	<div></div> 0.3210	<div></div> 0.4490
L	<div></div> 0.5130	<div></div> 0.5320

1.0

0.0

<0.0