



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 04:05 pm GMT

PDB ID : 8QPR  
EMDB ID : EMD-18560  
Title : SARS-CoV-2 S protein bound to human neutralising antibody UZGENT\_G5  
Authors : Remaut, H.; Reiter, D.; Vandenkerckhove, L.; Acar, D.D.; Witkowski, W.; Gerlo, S.  
Deposited on : 2023-10-03  
Resolution : 3.80 Å(reported)  
Based on initial model : 7K8V

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 : 1.8.4, CSD as541be (2020)  
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

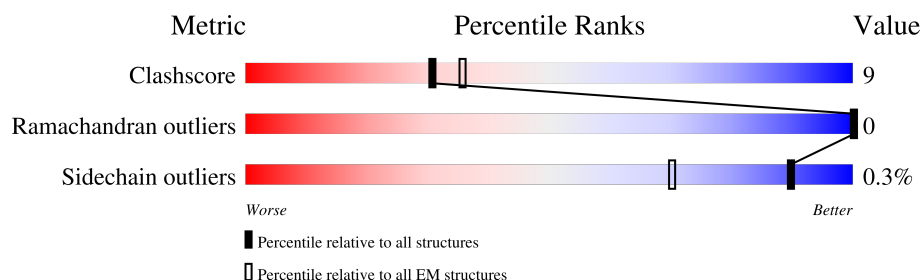
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1288	 12% 31% 7% 62%
2	D	216	 12% 37% 13% 50%
3	E	229	 12% 45% 8% 46%
4	B	2	 50% 50% 100%
4	F	2	 50% 50% 50%
4	a	2	 50% 50% 100%
5	G	3	 33% 67% 33%
5	c	3	 67% 67% 100%

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Mol	Chain	Length	Quality of chain
5	e	3	<div><div></div><div>33%</div><div></div><div>100%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5787 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 Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	491	Total	C	N	O	S	0	0
			3844	2481	636	712	15		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	engineered mutation	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	PRO	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	SER	-	expression tag	UNP P10104
A	1259	ALA	-	expression tag	UNP P10104
A	1260	TRP	-	expression tag	UNP P10104
A	1261	SER	-	expression tag	UNP P10104
A	1262	HIS	-	expression tag	UNP P10104
A	1263	PRO	-	expression tag	UNP P10104
A	1264	GLN	-	expression tag	UNP P10104
A	1265	PHE	-	expression tag	UNP P10104
A	1266	GLU	-	expression tag	UNP P10104
A	1267	LYS	-	expression tag	UNP P10104
A	1268	GLY	-	expression tag	UNP P10104
A	1269	GLY	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	GLY	-	expression tag	UNP P10104
A	1273	GLY	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	GLY	-	expression tag	UNP P10104
A	1278	GLY	-	expression tag	UNP P10104
A	1279	SER	-	expression tag	UNP P10104
A	1280	ALA	-	expression tag	UNP P10104
A	1281	TRP	-	expression tag	UNP P10104
A	1282	SER	-	expression tag	UNP P10104
A	1283	HIS	-	expression tag	UNP P10104
A	1284	PRO	-	expression tag	UNP P10104
A	1285	GLN	-	expression tag	UNP P10104
A	1286	PHE	-	expression tag	UNP P10104
A	1287	GLU	-	expression tag	UNP P10104
A	1288	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called IgG light chain - FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	109	Total	C	N	O	S	0	0
			803	500	136	164	3		

- Molecule 3 is a protein called IgG heavy chain - FAB.

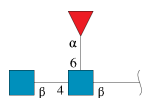
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	123	Total	C	N	O	S	0	0
			942	596	161	181	4		

- Molecule 4 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
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

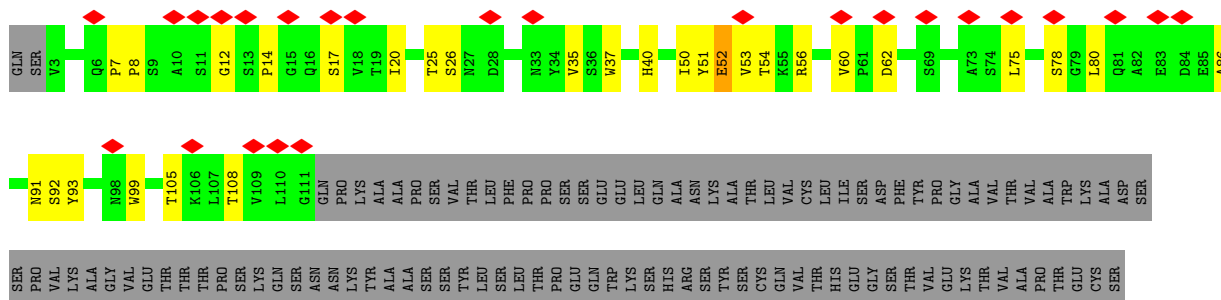
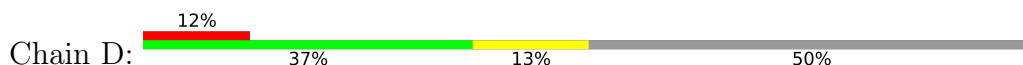


Mol	Chain	Residues	Atoms				AltConf	Trace
5	c	3	Total	C	N	O	0	0
			38	22	2	14		
5	G	3	Total	C	N	O	0	0
			38	22	2	14		
5	e	3	Total	C	N	O	0	0
			38	22	2	14		

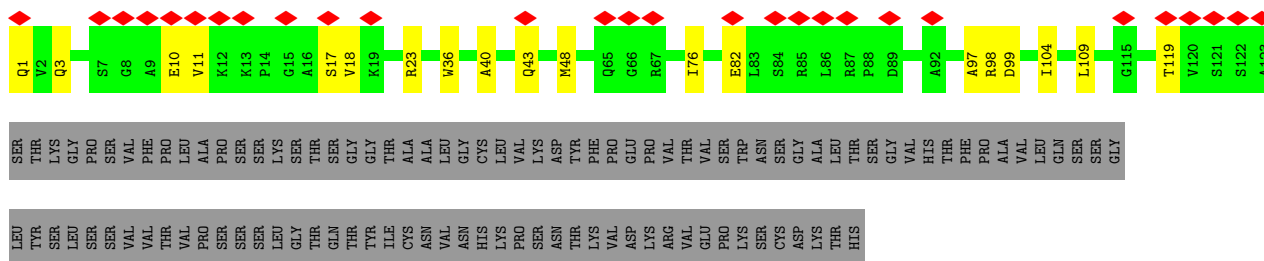


GLN PHE GLU GLY	ARG	ASP	THR	LYS	ASP	ASN	GLN PHE GLU GLY
		LEU	GLN	GLY	PRO	ASN	
GLY GLU GLY LEU	LYS	ASP	ARG	TYR	PRO	GLN	PHE
	GLY	ASP	ASN	ASN	GLU	ASN	SER
VAL LEU LEU LEU	TRP	SER	TYR	MET	VAL	ALA	ALA
	VAL	GLY	GLU	SER	GLN	GLY	ILE
PHE PHE PHE PHE	LEU	ILE	PRO	PHE	ILE	LYS	GLY
	LEU	ASN	GLN	ASN	PRO	ILE	LYS
THR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

- Molecule 2: IgG light chain - FAB



- Molecule 3: IgG heavy chain - FAB



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







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



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]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	161643	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.426	Depositor
Minimum map value	-1.926	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.369	Depositor
Map size ( $\text{\AA}$ )	449.27997, 449.27997, 449.27997	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.78, 0.78, 0.78	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/3947	0.53	1/5381 (0.0%)
2	D	0.31	0/824	0.57	0/1123
3	E	0.31	0/965	0.51	0/1316
All	All	0.36	0/5736	0.53	1/7820 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LEU	CA-CB-CG	5.74	128.49	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	TRP	Peptide
2	D	52	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3844	0	3667	66	0
2	D	803	0	755	20	0
3	E	942	0	916	11	0
4	B	28	0	25	0	0
4	F	28	0	25	0	0
4	a	28	0	25	0	0
5	G	38	0	34	3	0
5	c	38	0	34	0	0
5	e	38	0	34	0	0
All	All	5787	0	5515	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:VAL:HG12	2:D:54:THR:HG23	1.62	0.81
2:D:50:ILE:HD11	2:D:54:THR:HA	1.68	0.74
1:A:70:VAL:HA	1:A:76:THR:HG23	1.71	0.72
1:A:69:HIS:HB3	1:A:78:ARG:HD3	1.73	0.70
1:A:328:ARG:HD2	1:A:533:LEU:HB2	1.73	0.70
3:E:23:ARG:NH1	3:E:76:ILE:O	2.25	0.69
2:D:25:THR:HG22	2:D:26:SER:H	1.60	0.67
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.58	0.66
1:A:212:LEU:HD12	1:A:213:VAL:HG22	1.78	0.64
1:A:454:ARG:NH2	1:A:467:ASP:O	2.30	0.64
1:A:366:SER:O	1:A:370:ASN:ND2	2.31	0.64
1:A:213:VAL:HG23	1:A:215:ASP:H	1.64	0.63
2:D:14:PRO:HA	2:D:80:LEU:HD22	1.81	0.63
3:E:97:ALA:HB1	3:E:109:LEU:HB3	1.82	0.62
1:A:406:GLU:HG2	1:A:418:ILE:HD12	1.81	0.62
1:A:42:VAL:O	1:A:563:GLN:NE2	2.34	0.60
1:A:403:ARG:HD2	1:A:505:TYR:CD1	2.37	0.59
1:A:331:ASN:OD1	5:G:1:NAG:N2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:O	1:A:82:PRO:HD3	2.03	0.58
1:A:131:CYS:HB2	1:A:133:PHE:CE1	2.39	0.58
2:D:93:TYR:HD1	2:D:99:TRP:HE1	1.50	0.57
1:A:357:ARG:NE	1:A:394:ASN:OD1	2.26	0.57
1:A:489:TYR:CE1	3:E:104:ILE:HG23	2.39	0.57
3:E:11:VAL:HG22	3:E:119:THR:HB	1.87	0.57
1:A:131:CYS:HA	1:A:166:CYS:HB2	1.86	0.56
5:G:1:NAG:H61	5:G:2:NAG:HN2	1.71	0.56
2:D:91:ASN:OD1	2:D:92:SER:N	2.39	0.56
1:A:188:ASN:HA	1:A:209:PRO:HA	1.87	0.55
1:A:403:ARG:HG2	1:A:404:GLY:H	1.73	0.54
2:D:56:ARG:NE	2:D:60:VAL:O	2.40	0.54
2:D:56:ARG:NH1	2:D:62:ASP:OD1	2.41	0.54
1:A:489:TYR:HE1	3:E:104:ILE:HG23	1.74	0.53
2:D:37:TRP:HB2	2:D:50:ILE:HG22	1.91	0.53
1:A:130:VAL:O	1:A:166:CYS:HB2	2.09	0.52
1:A:417:LYS:HA	1:A:420:ASP:OD1	2.08	0.52
1:A:231:ILE:HD12	1:A:233:ILE:HG12	1.92	0.52
1:A:538:CYS:HA	1:A:551:VAL:HA	1.91	0.51
1:A:212:LEU:HD12	1:A:213:VAL:N	2.26	0.51
2:D:40:HIS:O	2:D:86:ALA:HB1	2.11	0.51
2:D:17:SER:HB3	2:D:78:SER:HA	1.94	0.50
1:A:110:LEU:HB3	1:A:135:PHE:HD2	1.76	0.50
3:E:40:ALA:HB3	3:E:43:GLN:HB2	1.93	0.50
1:A:130:VAL:HG12	1:A:168:PHE:HB3	1.94	0.50
1:A:409:GLN:NE2	1:A:416:GLY:HA3	2.27	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.49
1:A:99:ASN:O	1:A:102:ARG:NH2	2.43	0.49
1:A:421:TYR:CE2	1:A:457:ARG:HB3	2.48	0.49
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.94	0.49
2:D:7:PRO:O	2:D:105:THR:OG1	2.25	0.49
3:E:1:GLN:NE2	3:E:3:GLN:OE1	2.47	0.48
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.31	0.48
3:E:17:SER:OG	3:E:82:GLU:OE2	2.29	0.48
1:A:287:ASP:OD1	1:A:288:ALA:N	2.47	0.48
1:A:328:ARG:HH11	1:A:533:LEU:H	1.62	0.47
3:E:98:ARG:HG2	3:E:99:ASP:O	2.13	0.47
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.80	0.47
1:A:103:GLY:HA3	1:A:119:ILE:O	2.14	0.47
3:E:10:GLU:HG2	3:E:18:VAL:HG23	1.96	0.47
1:A:347:PHE:CE2	1:A:509:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LYS:NZ	1:A:390:LEU:HD11	2.30	0.47
1:A:83:VAL:HG12	1:A:239:GLN:HB2	1.97	0.47
1:A:328:ARG:NH1	1:A:533:LEU:H	2.13	0.47
2:D:35:VAL:HA	2:D:91:ASN:O	2.15	0.46
1:A:118:LEU:HB2	1:A:133:PHE:HE2	1.81	0.46
1:A:131:CYS:HA	1:A:166:CYS:CB	2.45	0.45
2:D:93:TYR:HD1	2:D:99:TRP:NE1	2.13	0.45
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.52	0.45
1:A:98:SER:OG	1:A:99:ASN:N	2.48	0.45
1:A:555:SER:OG	1:A:556:ASN:N	2.50	0.45
1:A:518:LEU:HD12	1:A:518:LEU:O	2.17	0.45
2:D:7:PRO:HA	2:D:8:PRO:HD3	1.88	0.45
2:D:12:GLY:N	2:D:108:THR:O	2.50	0.44
1:A:393:THR:HG22	1:A:394:ASN:HD22	1.81	0.44
2:D:51:TYR:HD2	2:D:52:GLU:HG2	1.83	0.44
1:A:342:PHE:HE2	1:A:434:ILE:HG21	1.83	0.44
1:A:20:THR:OG1	1:A:79:PHE:N	2.48	0.43
1:A:108:THR:O	1:A:237:ARG:NH2	2.50	0.43
1:A:403:ARG:HD2	1:A:505:TYR:HD1	1.80	0.43
2:D:20:ILE:HD11	2:D:105:THR:HB	1.99	0.43
1:A:403:ARG:HG2	1:A:404:GLY:N	2.32	0.43
1:A:393:THR:HB	1:A:517:LEU:HA	2.00	0.43
2:D:37:TRP:HB2	2:D:50:ILE:CG2	2.49	0.43
2:D:50:ILE:HG21	2:D:75:LEU:HD21	1.99	0.43
1:A:95:THR:O	1:A:95:THR:HG23	2.18	0.43
1:A:382:VAL:O	1:A:383:SER:OG	2.32	0.43
3:E:36:TRP:O	3:E:48:MET:HB2	2.19	0.43
1:A:437:ASN:OD1	1:A:438:SER:N	2.53	0.42
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.55	0.42
1:A:447:GLY:HA2	1:A:497:PHE:O	2.19	0.41
1:A:231:ILE:HG13	1:A:232:GLY:N	2.36	0.41
1:A:296:LEU:O	1:A:300:LYS:HG2	2.20	0.41
1:A:406:GLU:N	1:A:406:GLU:OE1	2.54	0.41
1:A:387:LEU:C	1:A:387:LEU:HD12	2.42	0.40
1:A:210:ILE:HD13	1:A:217:PRO:HG3	2.03	0.40
5:G:1:NAG:H61	5:G:3:FUC:O2	2.22	0.40
1:A:34:ARG:HD2	1:A:191:GLU:OE1	2.22	0.40
1:A:212:LEU:HD12	1:A:213:VAL:H	1.86	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	481/1288 (37%)	414 (86%)	67 (14%)	0	100	100
2	D	107/216 (50%)	96 (90%)	11 (10%)	0	100	100
3	E	121/229 (53%)	110 (91%)	11 (9%)	0	100	100
All	All	709/1733 (41%)	620 (87%)	89 (13%)	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	420/1116 (38%)	418 (100%)	2 (0%)	86	90
2	D	88/181 (49%)	88 (100%)	0	100	100
3	E	100/193 (52%)	100 (100%)	0	100	100
All	All	608/1490 (41%)	606 (100%)	2 (0%)	90	92

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

Mol	Chain	Res	Type
1	A	207	HIS
1	A	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

15 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	$\# Z  > 2$
4	NAG	B	1	1,4	14,14,15	0.60	1 (7%)	17,19,21	0.59	0
4	NAG	B	2	4	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	F	1	1,4	14,14,15	0.95	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	G	1	1,5	14,14,15	0.37	0	17,19,21	0.59	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.47	0
5	FUC	G	3	5	10,10,11	1.10	1 (10%)	14,14,16	1.18	2 (14%)
4	NAG	a	1	1,4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	a	2	4	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	c	1	1,5	14,14,15	0.36	0	17,19,21	0.56	0
5	NAG	c	2	5	14,14,15	0.27	0	17,19,21	0.42	0
5	FUC	c	3	5	10,10,11	0.69	0	14,14,16	0.95	0
5	NAG	e	1	5,3	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
5	NAG	e	2	5	14,14,15	0.53	0	17,19,21	0.96	2 (11%)
5	FUC	e	3	5	10,10,11	0.63	0	14,14,16	1.15	2 (14%)

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
4	NAG	B	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
4	NAG	a	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	FUC	c	3	5	-	-	0/1/1/1
5	NAG	e	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	4/6/23/26	0/1/1/1
5	FUC	e	3	5	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-3.42	1.38	1.43
5	G	3	FUC	C1-C2	2.36	1.57	1.52
4	B	1	NAG	O5-C1	-2.15	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	3	FUC	C1-O5-C5	2.70	118.89	112.78
5	G	3	FUC	O2-C2-C1	2.50	114.28	109.15
5	e	2	NAG	C3-C4-C5	2.40	114.52	110.24
5	e	2	NAG	C1-O5-C5	2.39	115.44	112.19
4	F	1	NAG	C3-C4-C5	2.28	114.31	110.24
5	G	3	FUC	O5-C5-C4	2.28	113.61	109.52
5	e	3	FUC	O5-C5-C4	2.20	113.46	109.52
5	e	1	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

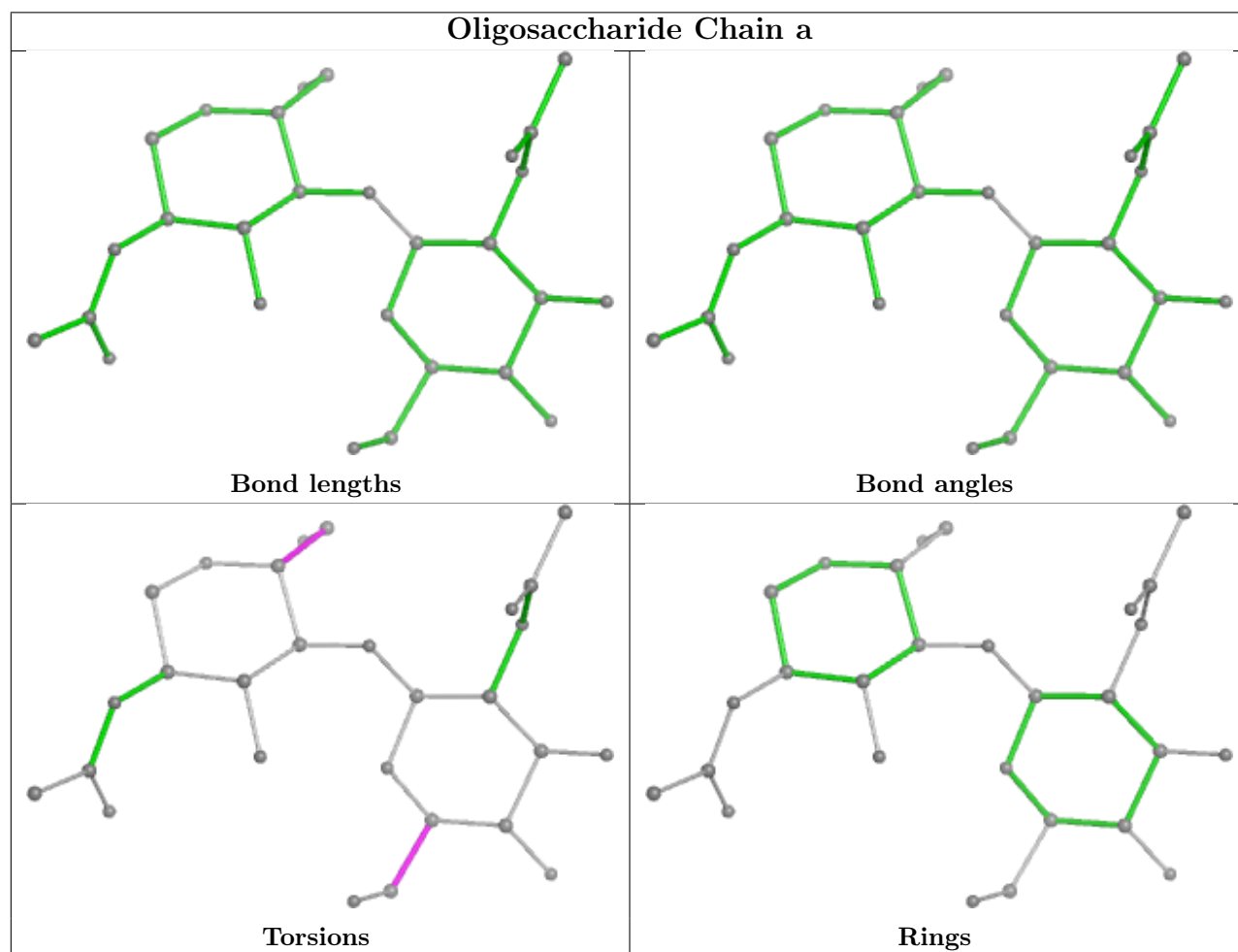
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
5	e	1	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
5	e	2	NAG	C8-C7-N2-C2
5	e	2	NAG	O7-C7-N2-C2
4	B	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
5	e	2	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
5	c	1	NAG	C1-C2-N2-C7
5	e	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C1-C2-N2-C7
4	B	1	NAG	C3-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
5	c	1	NAG	C3-C2-N2-C7
4	B	1	NAG	C1-C2-N2-C7

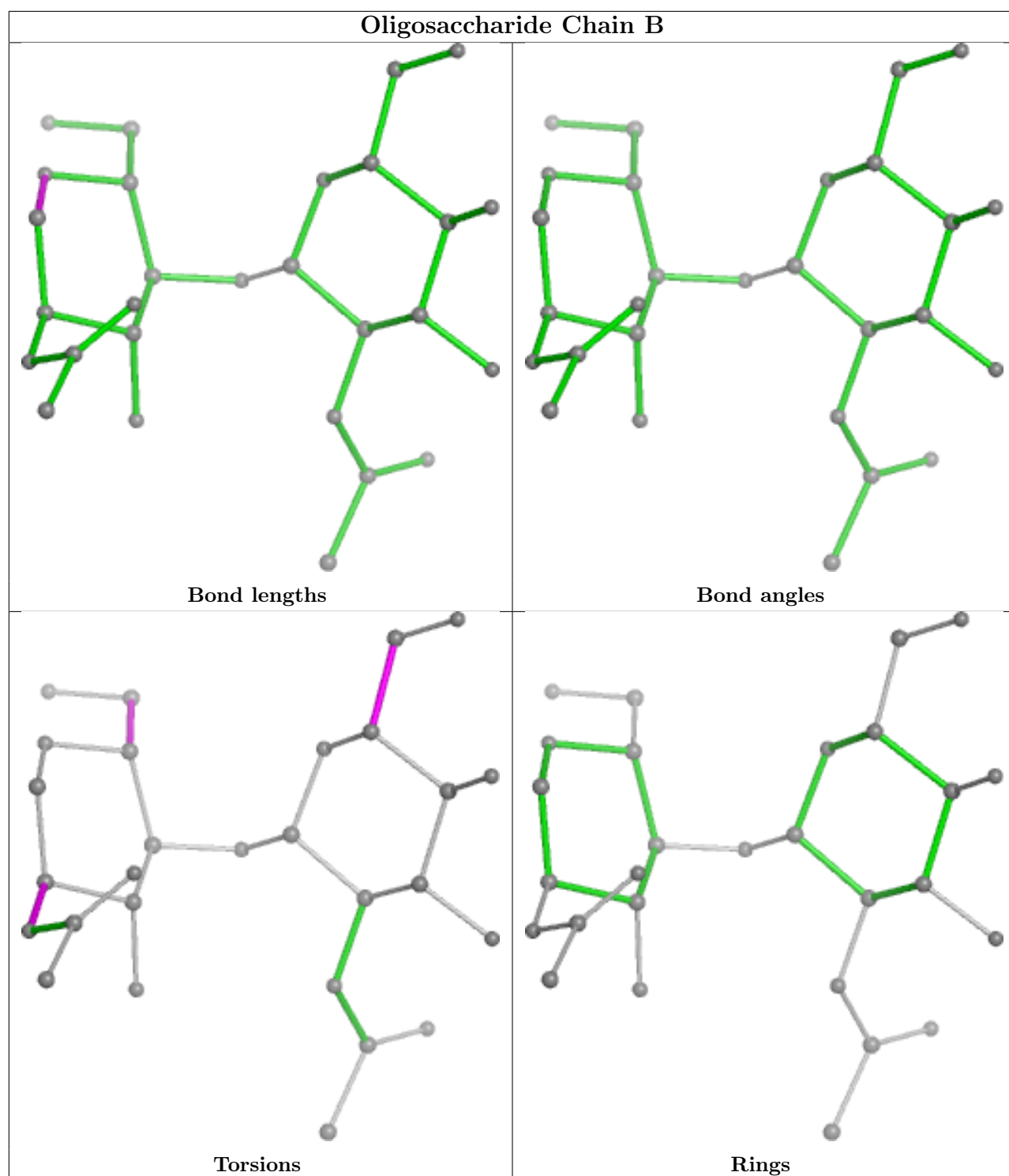
There are no ring outliers.

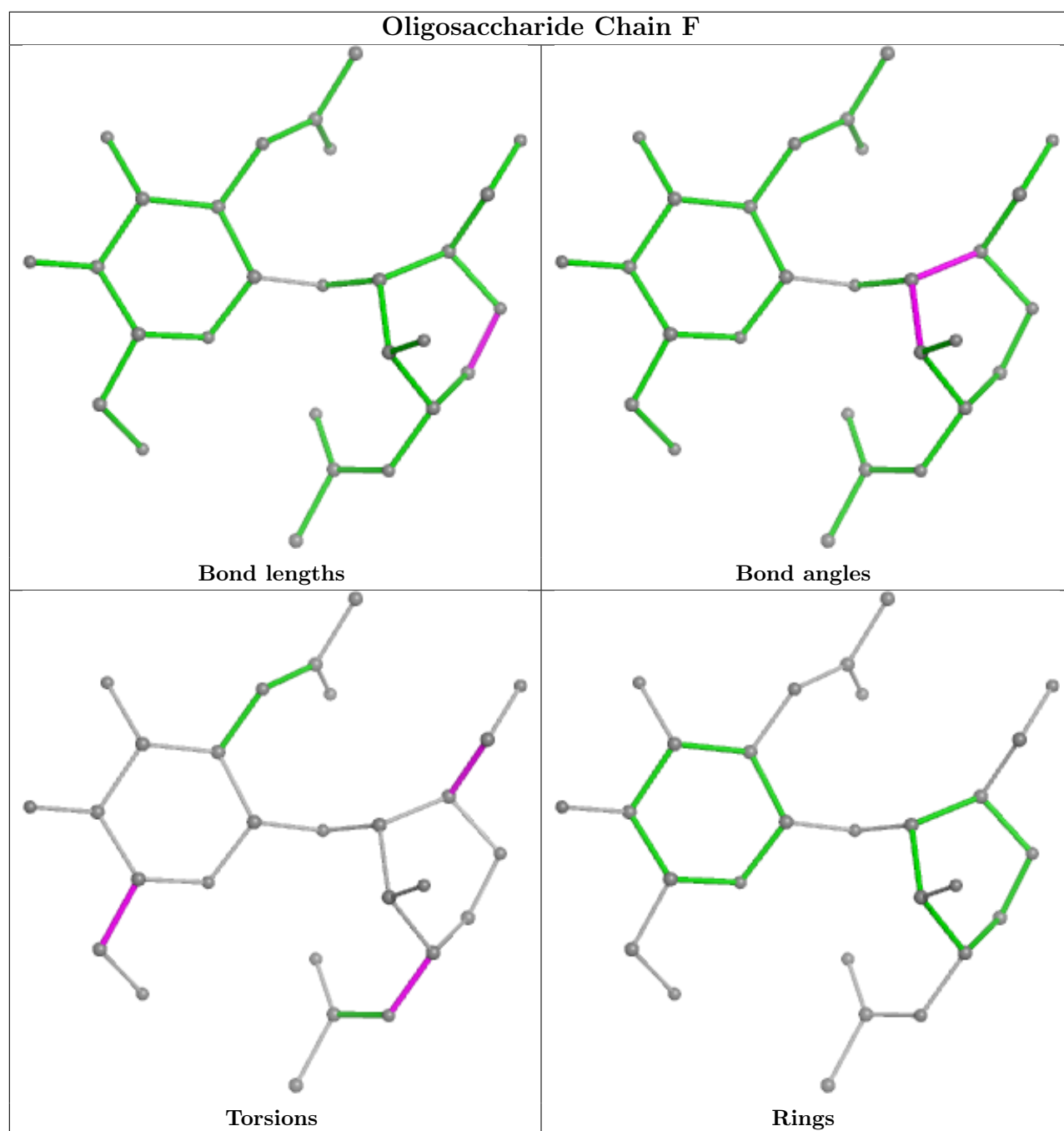
3 monomers are involved in 3 short contacts:

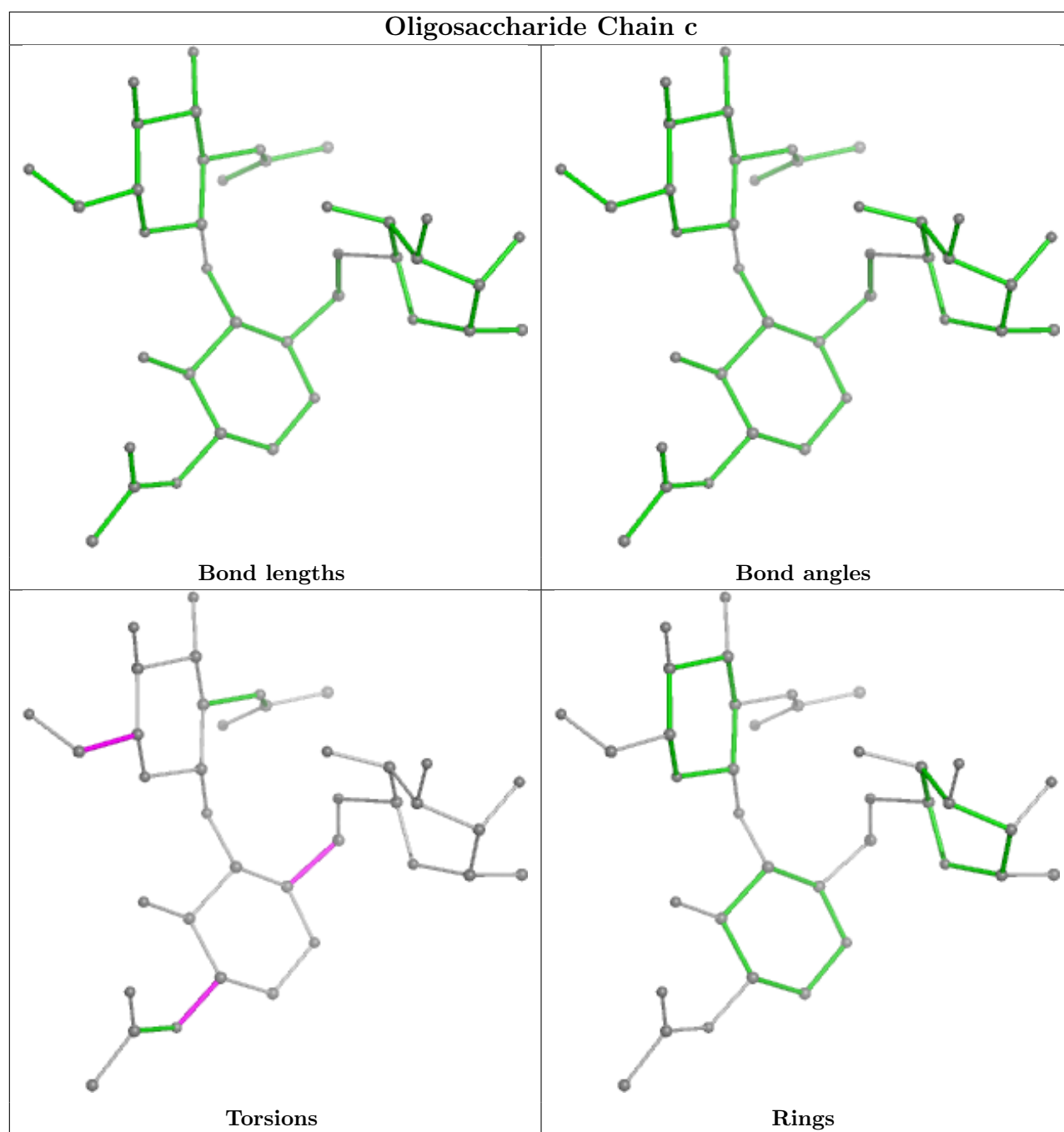
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	1	0
5	G	3	FUC	1	0
5	G	1	NAG	3	0

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

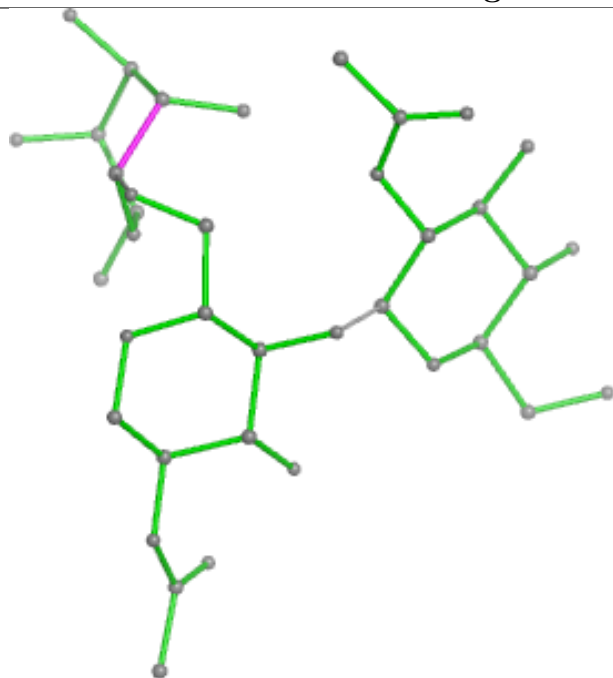




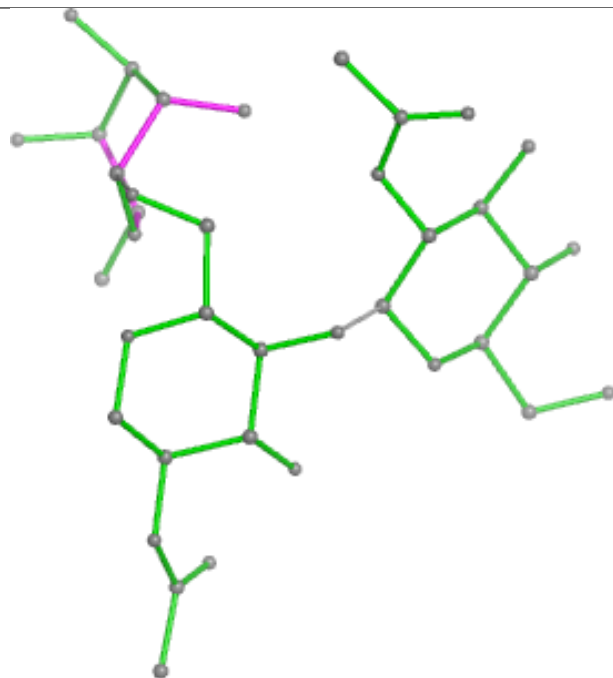




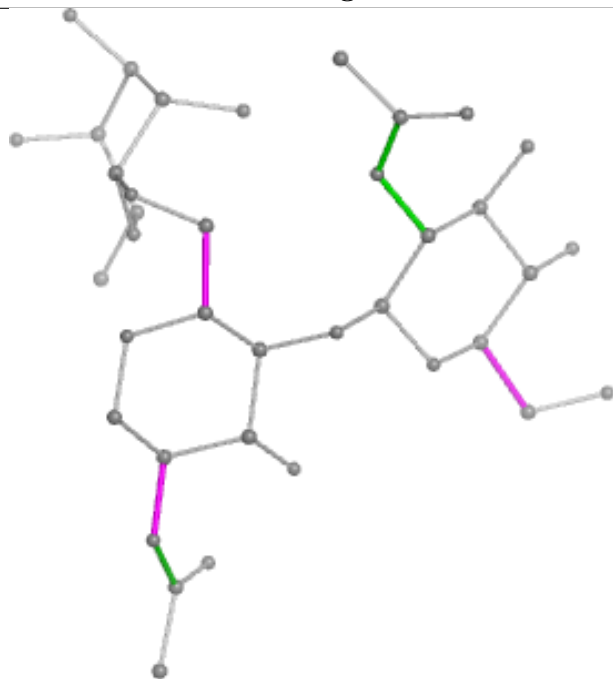
## Oligosaccharide Chain G



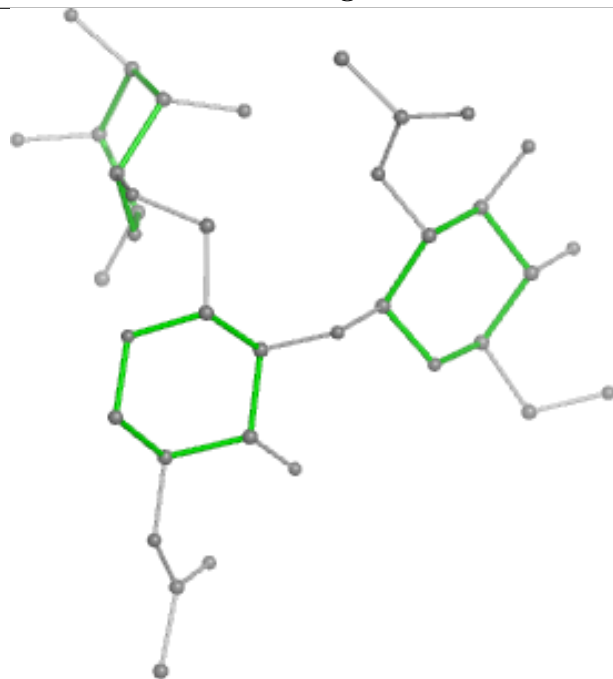
Bond lengths



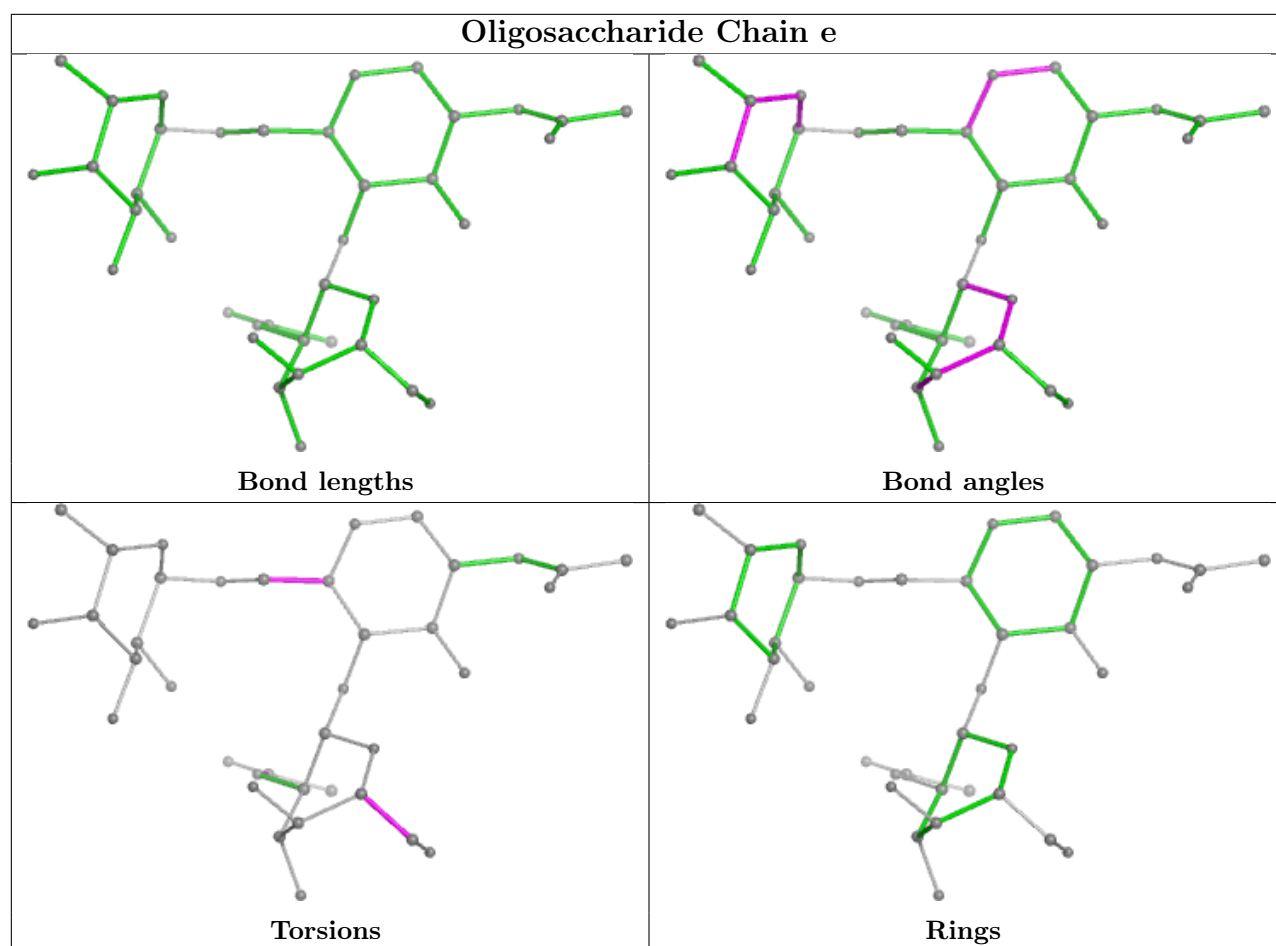
Bond angles



Torsions



Rings



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



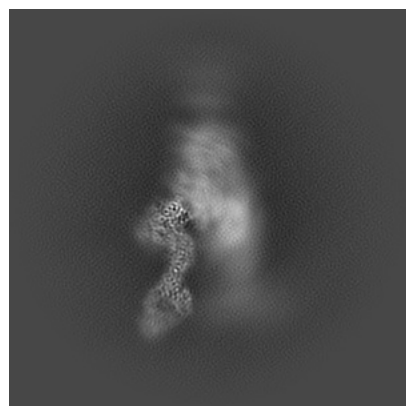
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18560. These allow visual inspection of the internal detail of the map and identification of artifacts.

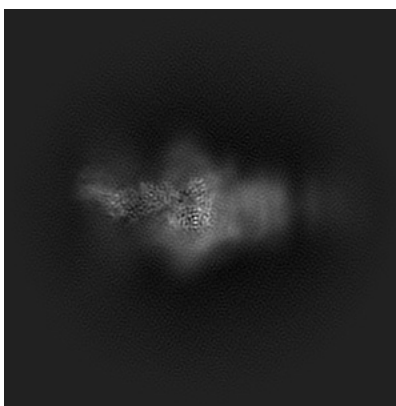
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

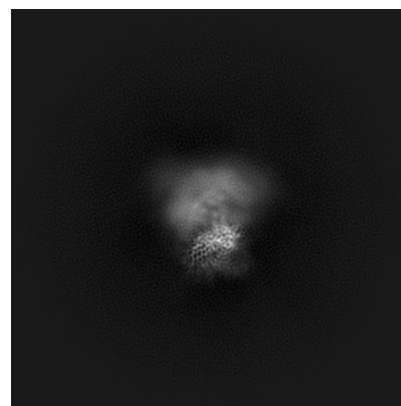
#### 6.1.1 Primary map



X

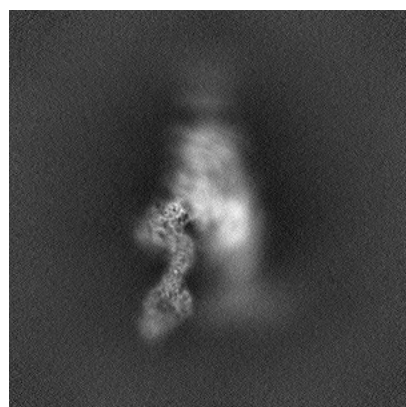


Y

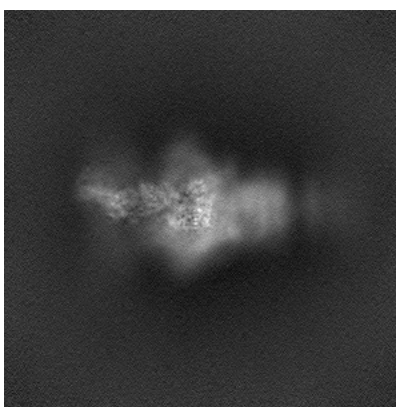


Z

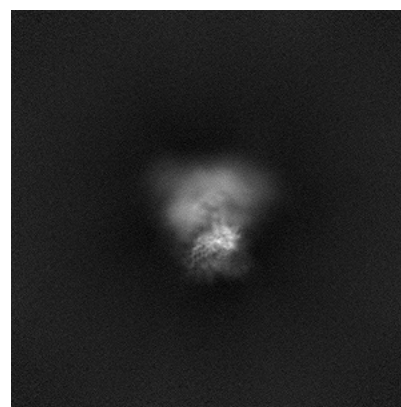
#### 6.1.2 Raw map



X



Y

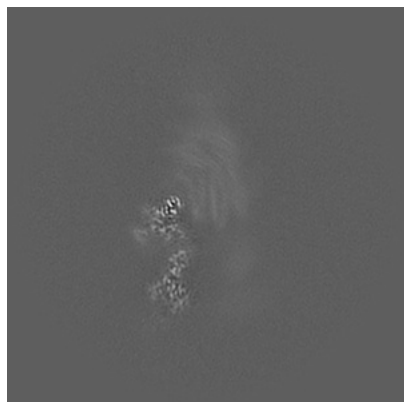


Z

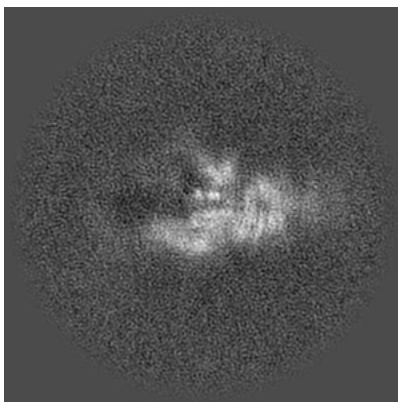
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

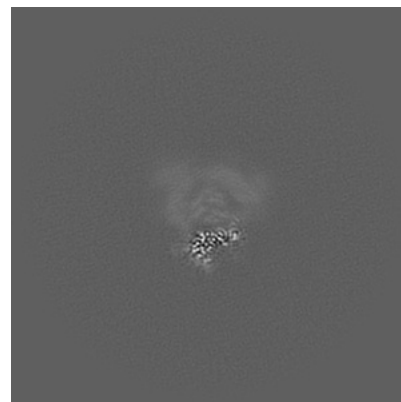
### 6.2.1 Primary map



X Index: 288



Y Index: 288

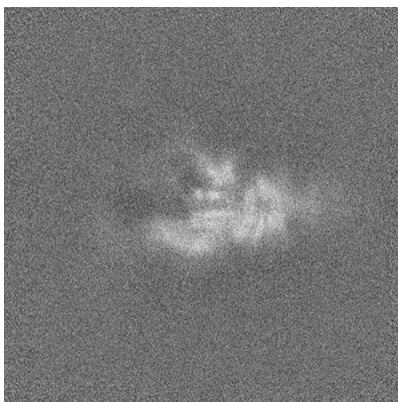


Z Index: 288

### 6.2.2 Raw map



X Index: 288



Y Index: 288

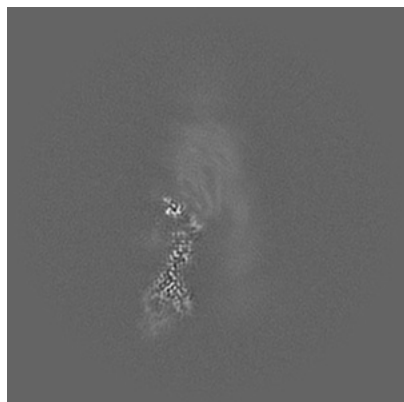


Z Index: 288

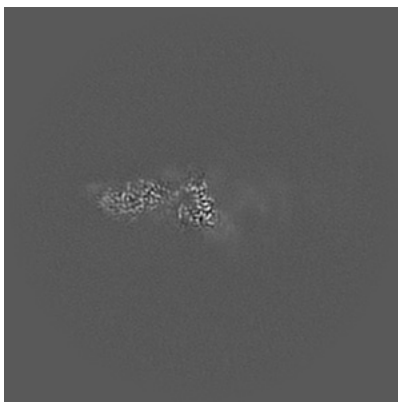
The images above show central slices of the map in three orthogonal directions.

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

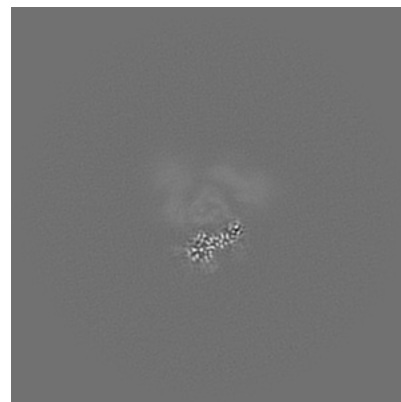
### 6.3.1 Primary map



X Index: 303



Y Index: 241

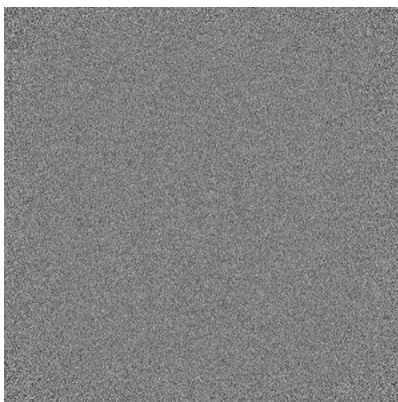


Z Index: 280

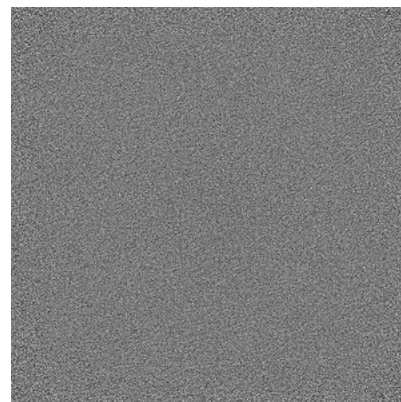
### 6.3.2 Raw map



X Index: 298



Y Index: 0

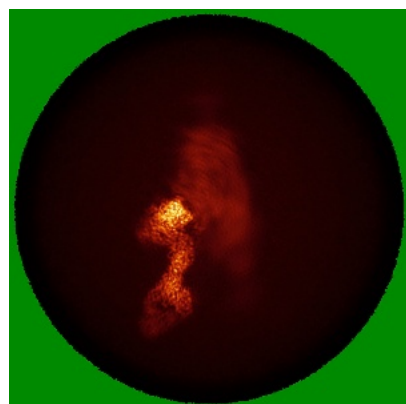


Z Index: 575

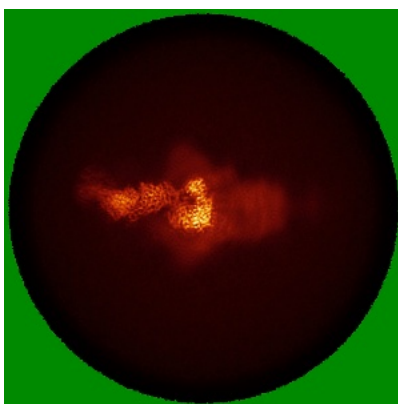
The images above show the largest variance slices of the map in three orthogonal directions.

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

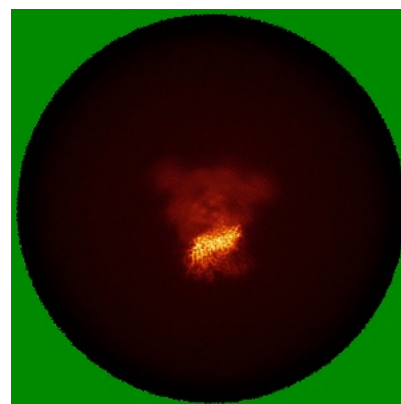
### 6.4.1 Primary map



X



Y

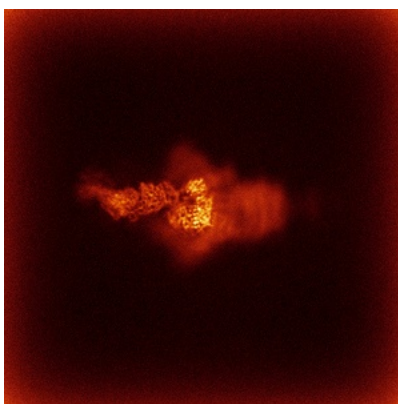


Z

### 6.4.2 Raw map



X



Y



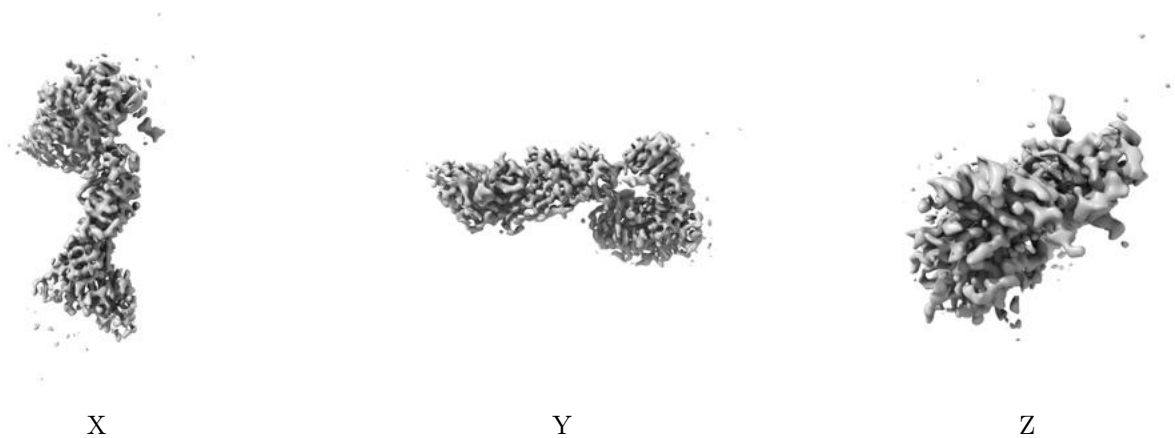
Z

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.



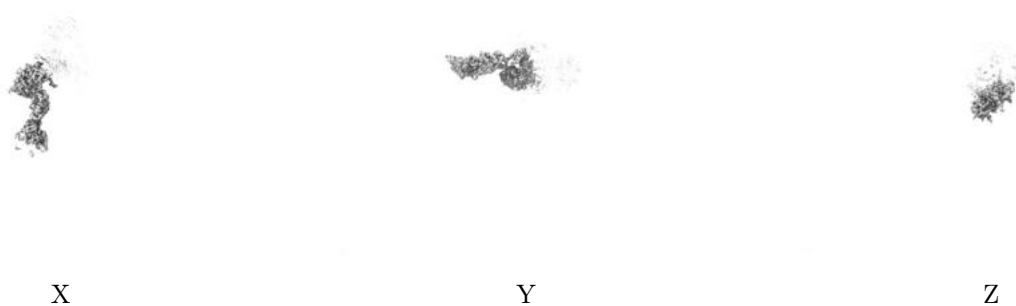
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.369. 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.

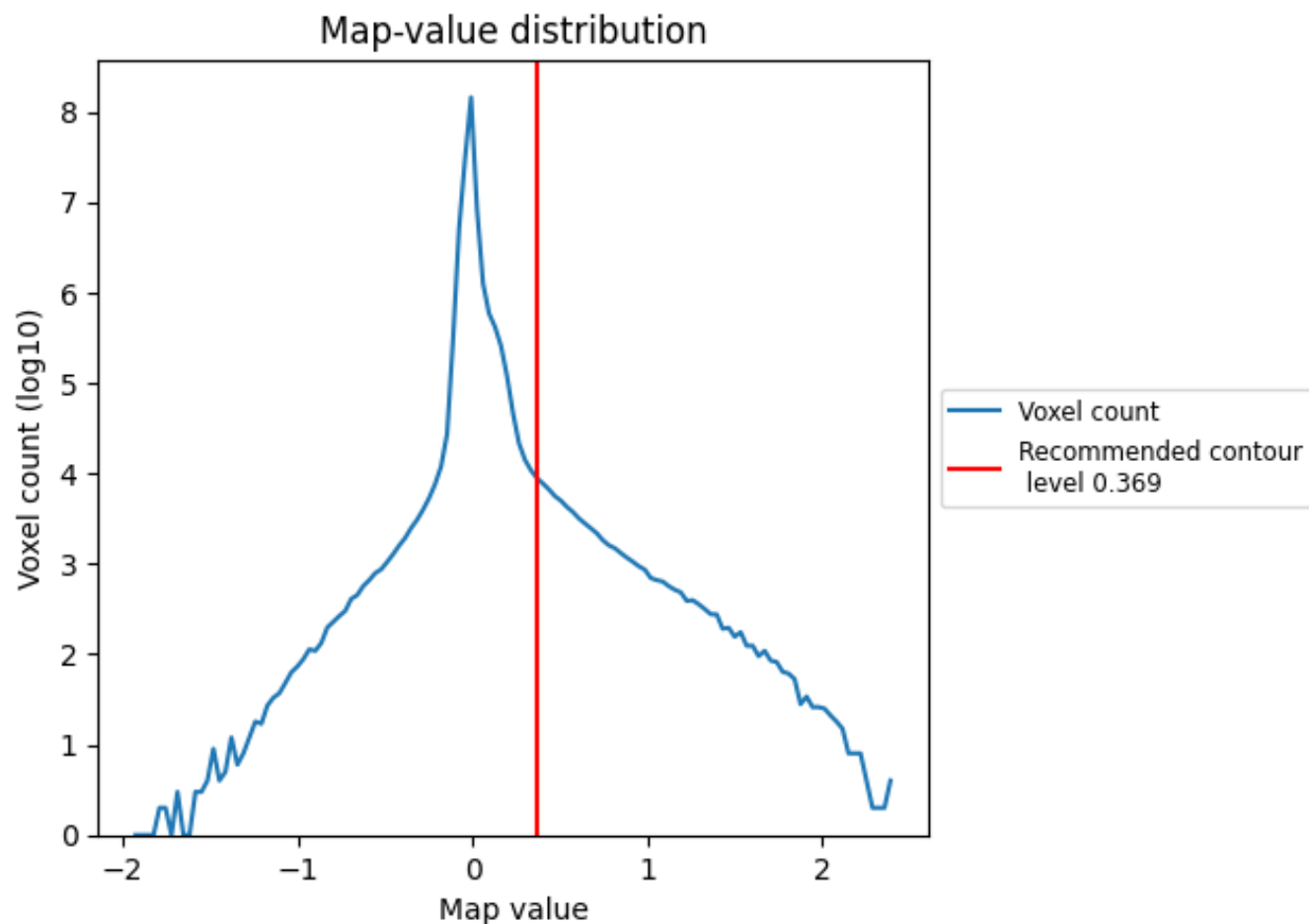
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

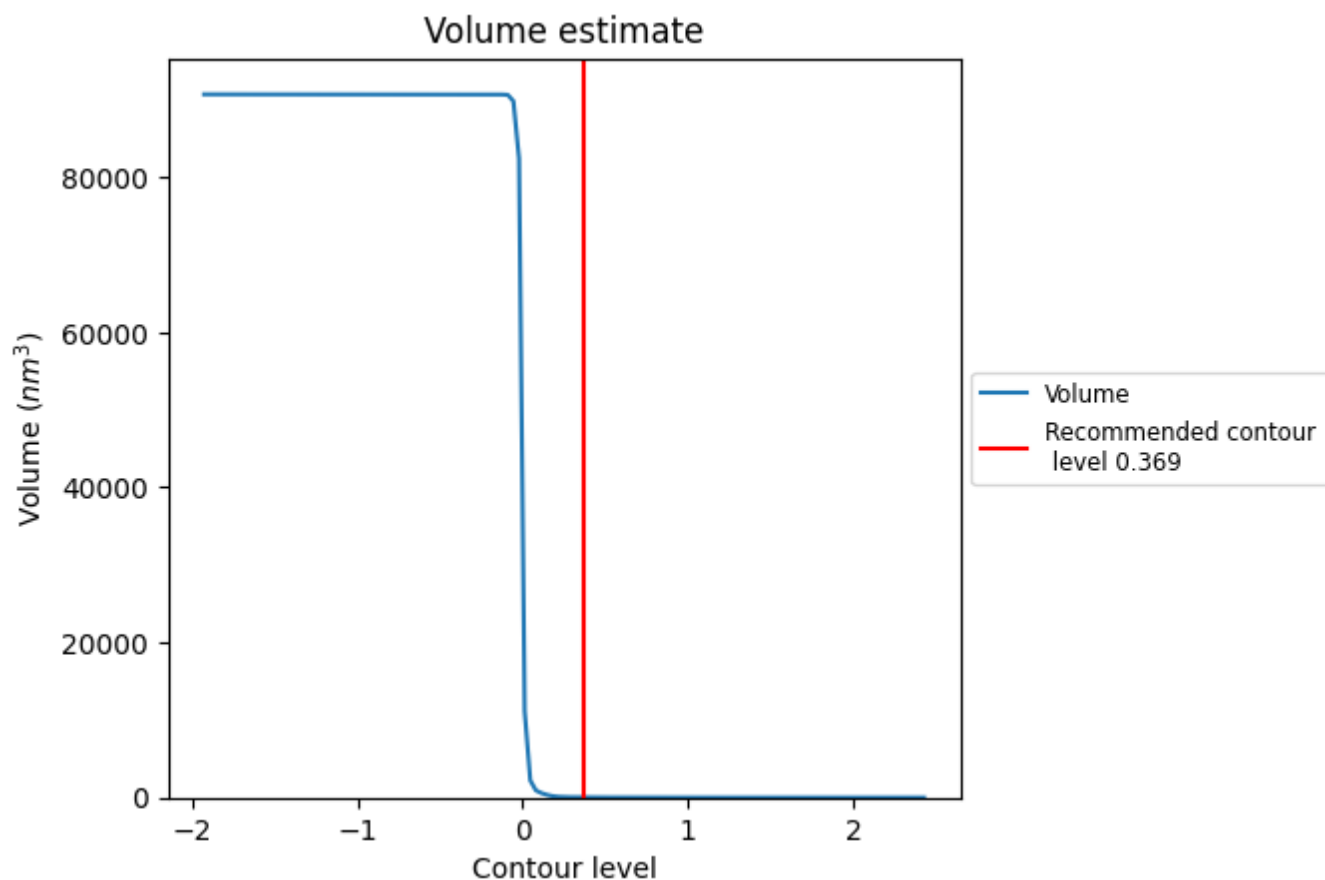
This section contains the results of statistical analysis of the map.

### 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.

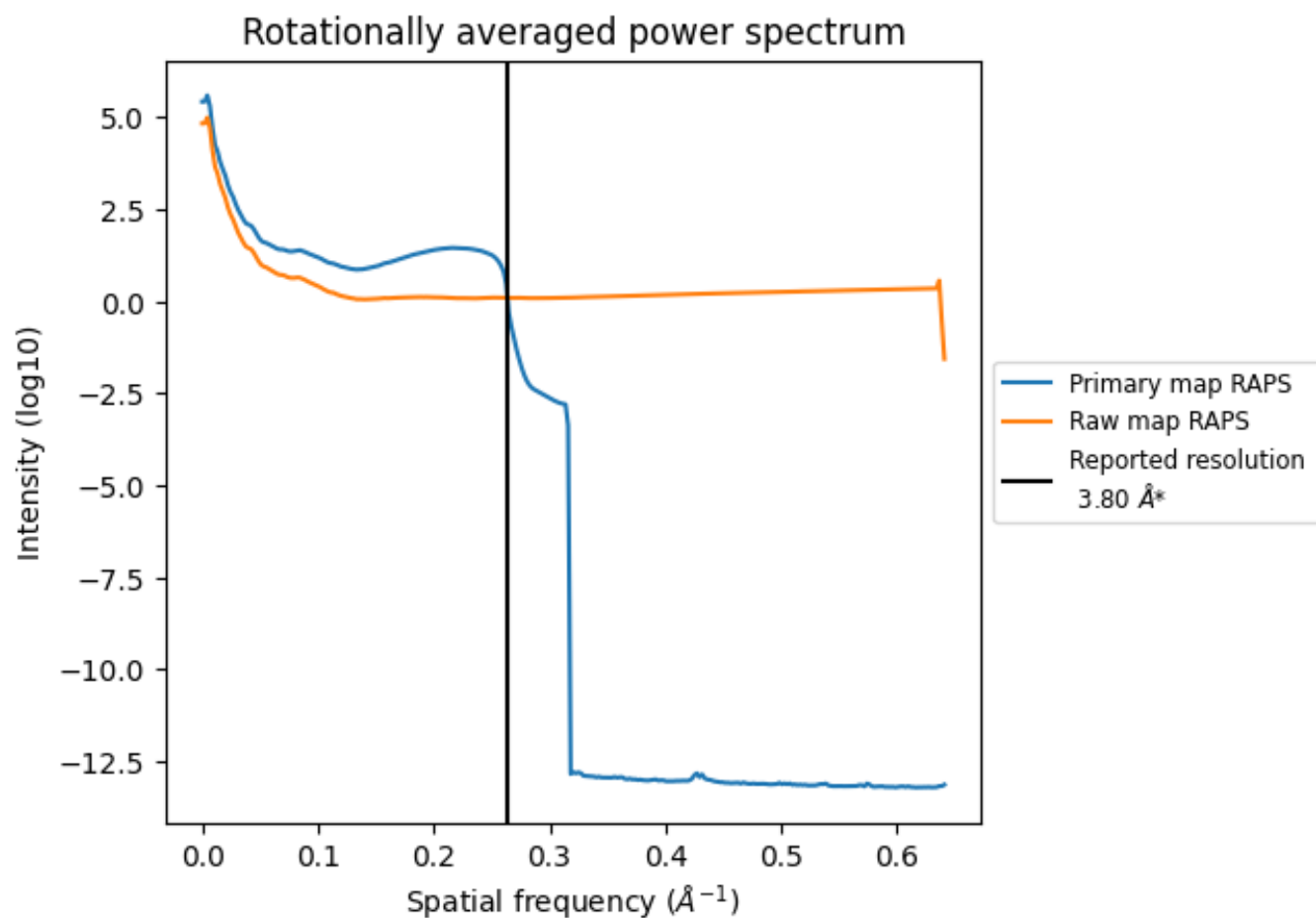
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm<sup>3</sup>; this corresponds to an approximate mass of 30 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 ⓘ



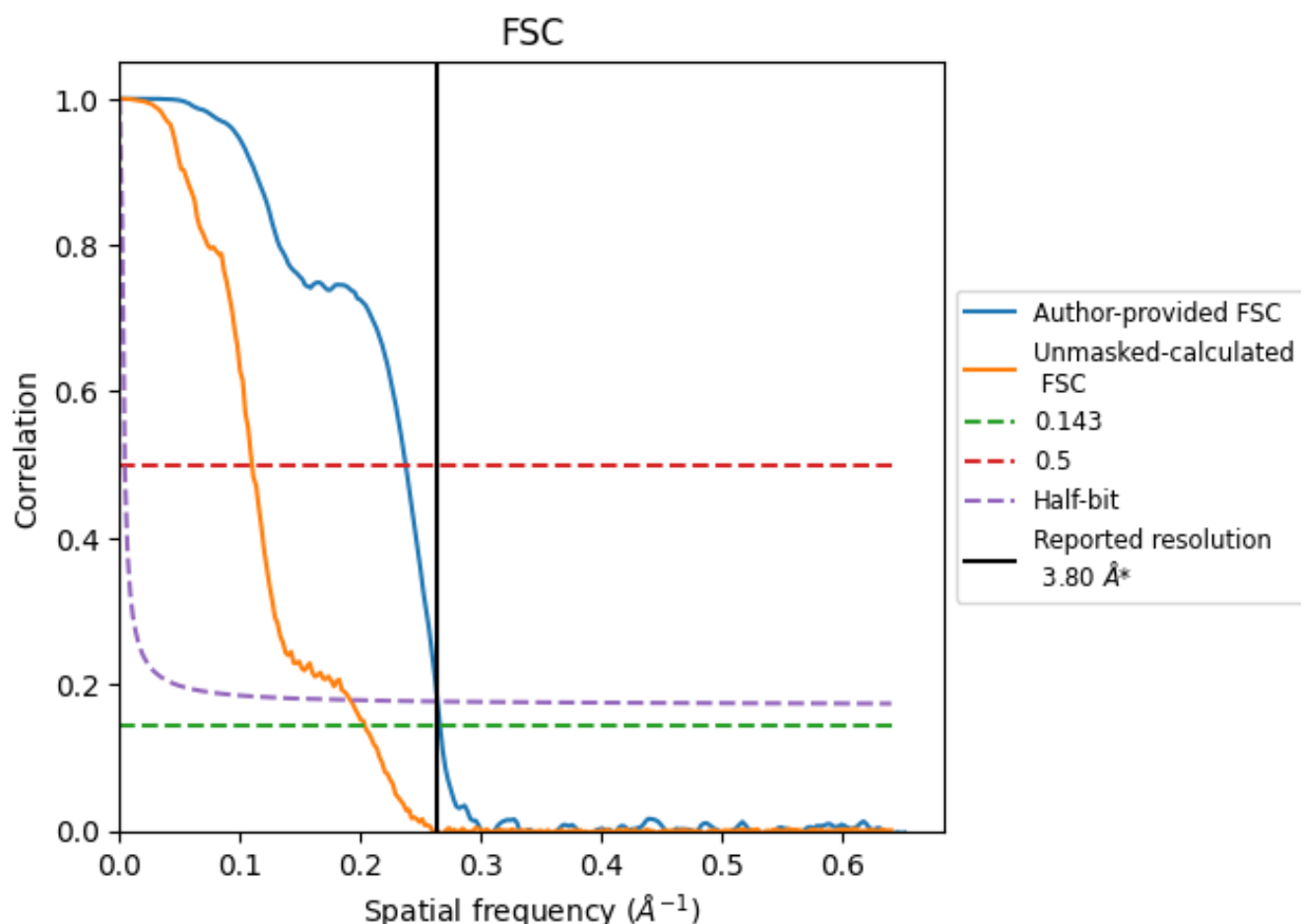
\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>



## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

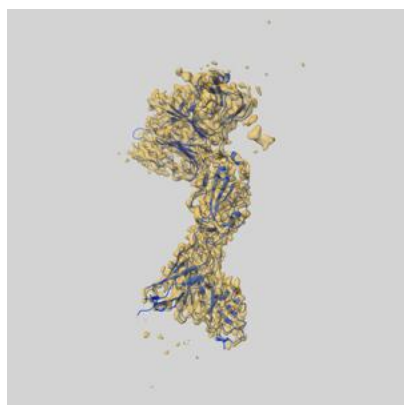
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.21	3.79
Unmasked-calculated*	4.90	9.09	5.22

\*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 4.90 differs from the reported value 3.8 by more than 10 %

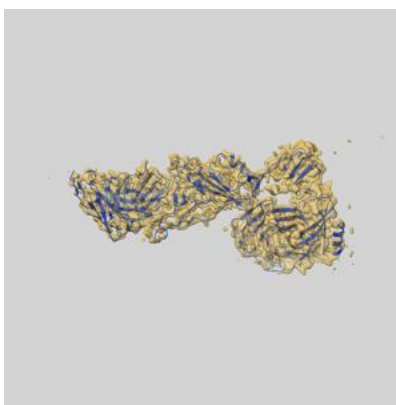
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18560 and PDB model 8QPR. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

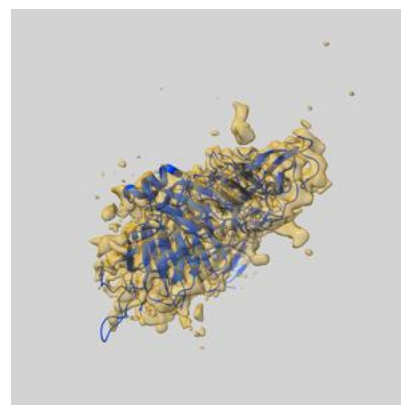
### 9.1 Map-model overlay [i](#)



X



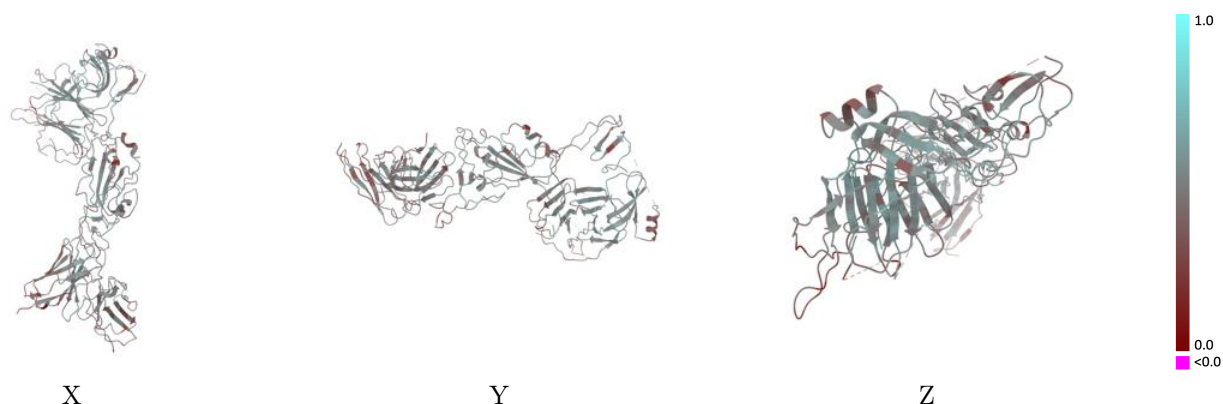
Y



Z

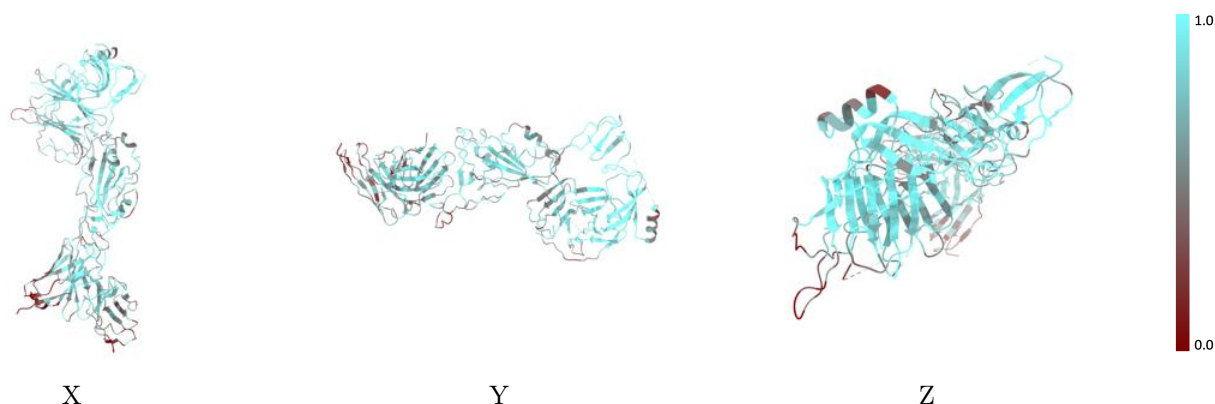
The images above show the 3D surface view of the map at the recommended contour level 0.369 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



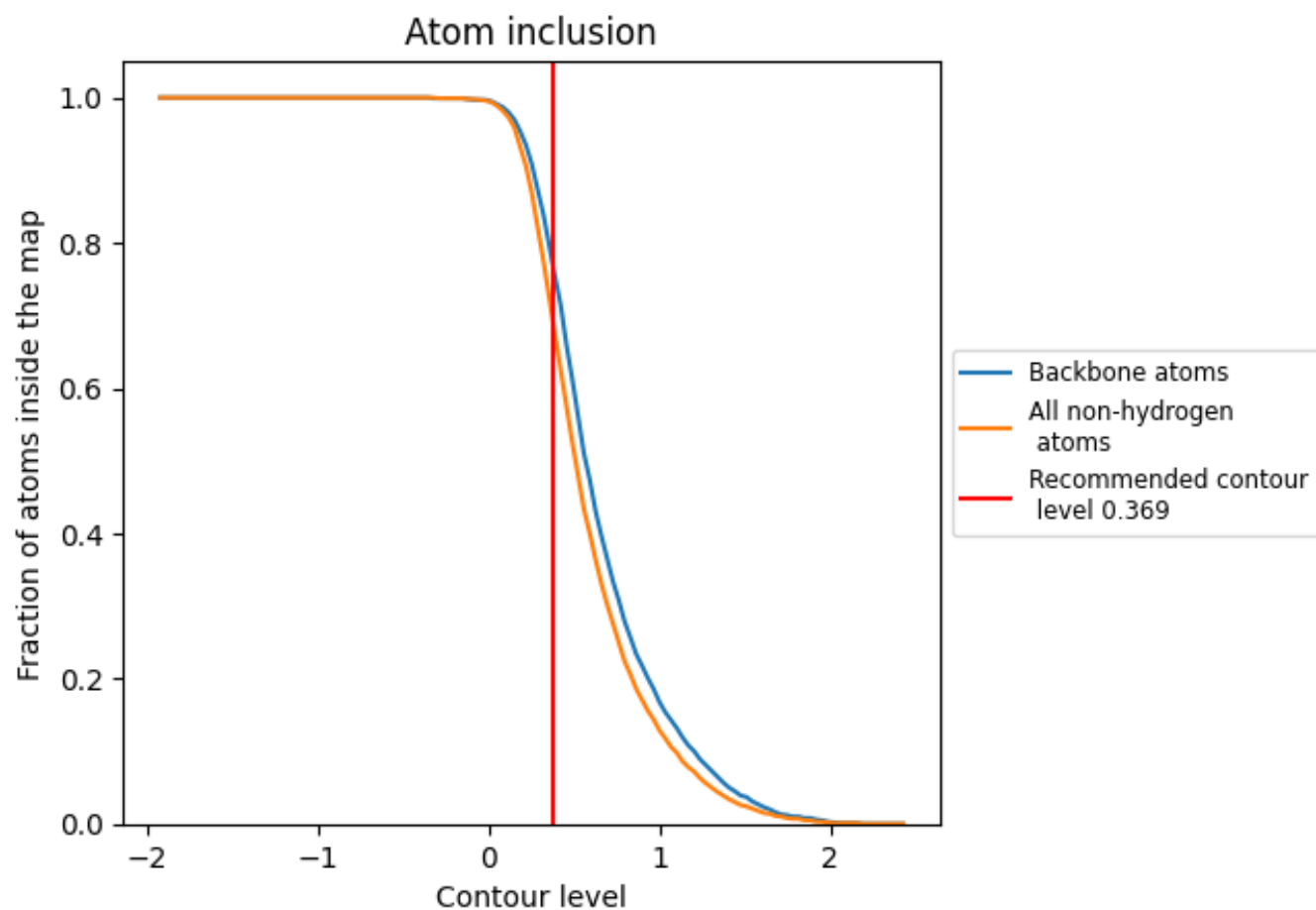
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.369).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.369) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6990	<div></div> 0.4690
A	<div></div> 0.7530	<div></div> 0.4830
B	<div></div> 0.2500	<div></div> 0.3560
D	<div></div> 0.5870	<div></div> 0.4350
E	<div></div> 0.6280	<div></div> 0.4500
F	<div></div> 0.2860	<div></div> 0.4040
G	<div></div> 0.6320	<div></div> 0.4260
a	<div></div> 0.5360	<div></div> 0.4420
c	<div></div> 0.3420	<div></div> 0.4030
e	<div></div> 0.5530	<div></div> 0.4970

1.0

0.0

<0.0