



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:14 AM UTC

PDB ID : 9DAK / pdb_00009dak
EMDB ID : EMD-46691
Title : Merbecovirus PnNL2018B Spike glycoprotein RBD bound to the P. Nathusii ACE2
Authors : Park, Y.J.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-08-22
Resolution : 2.40 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

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

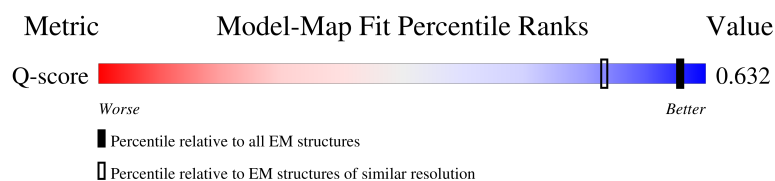
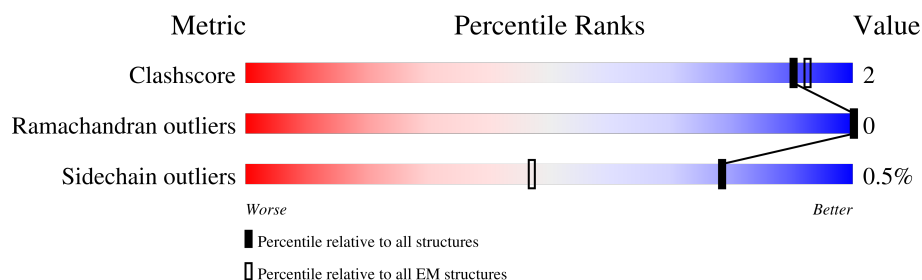
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	891	
2	B	315	
3	C	3	
3	F	3	

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Mol	Chain	Length	Quality of chain
4	D	2	50%100%
4	E	2	50%100%
4	H	2	50%50%
5	G	3	33%67%
5	I	3	33%67%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7303 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.

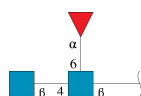
- Molecule 1 is a protein called ACE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	707	Total	C	N	O	S	0	0
			5544	3585	950	978	31		

- Molecule 2 is a protein called Spike glycoprotein receptor binding domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	192	Total	C	N	O	S	0	0
			1320	836	236	240	8		

- Molecule 3 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
3	C	3	Total	C	N	O	0	0
			38	22	2	14		
3	F	3	Total	C	N	O	0	0
			38	22	2	14		

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



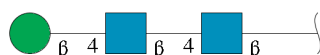
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

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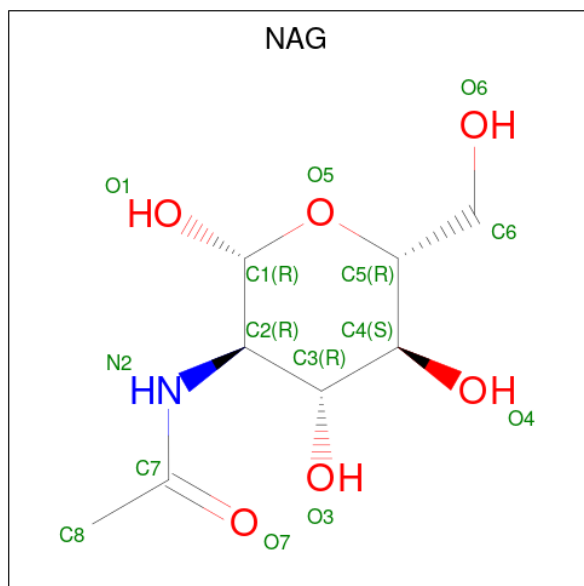
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	139	Total	O	0
			139	139	
8	B	5	Total	O	0
			5	5	

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



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



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





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1555546	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.309	Depositor
Minimum map value	-1.747	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	320.352, 320.352, 320.352	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0011, 1.0011, 1.0011	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.58	0/5699	0.84	55/7751 (0.7%)
2	B	0.56	0/1354	1.14	27/1855 (1.5%)
All	All	0.58	0/7053	0.91	82/9606 (0.9%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	517	LEU	CD1-CG-CD2	9.95	132.69	110.80
1	A	138	ASN	CA-C-N	7.79	127.51	119.56
1	A	138	ASN	C-N-CA	7.79	127.51	119.56
1	A	257	SER	CA-C-N	7.49	127.20	119.56
1	A	257	SER	C-N-CA	7.49	127.20	119.56
2	B	392	GLY	CA-C-N	7.44	127.44	119.78
2	B	392	GLY	C-N-CA	7.44	127.44	119.78
1	A	537	GLY	CA-C-N	7.28	127.26	119.76
1	A	537	GLY	C-N-CA	7.28	127.26	119.76
1	A	489	GLU	CA-C-N	7.17	127.17	119.28
1	A	489	GLU	C-N-CA	7.17	127.17	119.28
2	B	430	THR	CA-C-N	7.07	126.77	119.56
2	B	430	THR	C-N-CA	7.07	126.77	119.56
2	B	394	VAL	CA-C-N	7.01	127.00	119.78
2	B	394	VAL	C-N-CA	7.01	127.00	119.78
2	B	531	LYS	CA-C-N	6.94	127.23	119.32
2	B	531	LYS	C-N-CA	6.94	127.23	119.32
2	B	471	LYS	CA-C-N	6.93	126.85	119.85
2	B	471	LYS	C-N-CA	6.93	126.85	119.85
1	A	428	TYR	CA-C-N	6.64	126.56	119.85
1	A	428	TYR	C-N-CA	6.64	126.56	119.85
1	A	414	THR	CA-C-N	6.55	127.07	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	THR	C-N-CA	6.55	127.07	119.47
1	A	335	GLU	CA-C-N	6.50	126.45	119.76
1	A	335	GLU	C-N-CA	6.50	126.45	119.76
2	B	529	ARG	CA-C-N	6.47	126.44	119.78
2	B	529	ARG	C-N-CA	6.47	126.44	119.78
2	B	494	ASN	CA-C-N	6.47	126.38	119.85
2	B	494	ASN	C-N-CA	6.47	126.38	119.85
2	B	563	ASP	CA-C-N	6.45	126.40	119.76
2	B	563	ASP	C-N-CA	6.45	126.40	119.76
2	B	458	LEU	CA-C-N	6.41	126.36	119.76
2	B	458	LEU	C-N-CA	6.41	126.36	119.76
1	A	388	GLN	CA-C-N	6.29	126.31	119.89
1	A	388	GLN	C-N-CA	6.29	126.31	119.89
1	A	252	TYR	CA-C-N	6.25	126.19	119.76
1	A	252	TYR	C-N-CA	6.25	126.19	119.76
2	B	575	GLU	CA-C-N	6.23	126.20	119.78
2	B	575	GLU	C-N-CA	6.23	126.20	119.78
2	B	520	PHE	CA-C-N	6.23	126.14	119.85
2	B	520	PHE	C-N-CA	6.23	126.14	119.85
2	B	396	GLN	CA-C-N	6.22	126.69	119.47
2	B	396	GLN	C-N-CA	6.22	126.69	119.47
1	A	324	THR	CA-C-N	6.17	126.35	119.32
1	A	324	THR	C-N-CA	6.17	126.35	119.32
1	A	468	ILE	CA-C-N	6.17	126.14	120.03
1	A	468	ILE	C-N-CA	6.17	126.14	120.03
1	A	694	ILE	CA-C-N	6.15	126.17	119.90
1	A	694	ILE	C-N-CA	6.15	126.17	119.90
1	A	135	ASN	CA-C-N	6.10	125.78	119.56
1	A	135	ASN	C-N-CA	6.10	125.78	119.56
1	A	84	PHE	CA-C-N	6.07	126.42	119.93
1	A	84	PHE	C-N-CA	6.07	126.42	119.93
1	A	564	LYS	CA-C-N	6.01	126.03	119.90
1	A	564	LYS	C-N-CA	6.01	126.03	119.90
1	A	283	VAL	CA-C-N	5.96	127.29	119.84
1	A	283	VAL	C-N-CA	5.96	127.29	119.84
1	A	686	SER	CA-C-N	5.87	126.01	119.32
1	A	686	SER	C-N-CA	5.87	126.01	119.32
1	A	345	HIS	CA-C-N	5.86	126.05	119.90
1	A	345	HIS	C-N-CA	5.86	126.05	119.90
1	A	450	LEU	CA-C-N	5.86	125.53	119.56
1	A	450	LEU	C-N-CA	5.86	125.53	119.56
1	A	262	LEU	CA-C-N	5.64	125.92	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LEU	C-N-CA	5.64	125.92	119.83
1	A	582	LYS	CA-C-N	5.60	125.70	119.32
1	A	582	LYS	C-N-CA	5.60	125.70	119.32
1	A	610	SER	CA-C-N	5.54	126.77	119.84
1	A	610	SER	C-N-CA	5.54	126.77	119.84
1	A	177	ARG	CA-C-N	5.40	124.92	119.19
1	A	177	ARG	C-N-CA	5.40	124.92	119.19
1	A	213	ASP	CB-CA-C	-5.34	110.40	116.54
1	A	491	LEU	CA-C-N	5.32	125.49	119.90
1	A	491	LEU	C-N-CA	5.32	125.49	119.90
1	A	234	LYS	CA-C-N	5.24	125.04	119.28
1	A	234	LYS	C-N-CA	5.24	125.04	119.28
2	B	510	GLN	CA-C-N	5.21	125.74	120.38
2	B	510	GLN	C-N-CA	5.21	125.74	120.38
1	A	499	ASP	CA-C-N	5.04	124.83	119.28
1	A	499	ASP	C-N-CA	5.04	124.83	119.28
1	A	589	LYS	CA-C-N	5.00	124.78	119.28
1	A	589	LYS	C-N-CA	5.00	124.78	119.28

There are no chirality outliers.

There are no planarity outliers.

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	5544	0	5165	20	0
2	B	1320	0	1083	2	0
3	C	38	0	34	0	0
3	F	38	0	34	0	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	H	28	0	25	0	0
5	G	39	0	34	0	0
5	I	39	0	34	0	0
6	A	42	0	39	5	0
6	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	A	139	0	0	5	0
8	B	5	0	0	1	0
All	All	7303	0	6511	22	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 2.

All (22) 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:27:ARG:NH1	6:A:901:NAG:H61	1.66	1.10
1:A:27:ARG:HH12	6:A:901:NAG:H61	1.17	0.98
1:A:27:ARG:HH12	6:A:901:NAG:C6	1.87	0.87
1:A:350:ASP:OD1	8:A:1001:HOH:O	1.93	0.85
1:A:27:ARG:NH1	6:A:901:NAG:C6	2.44	0.81
2:B:523:PHE:O	8:B:801:HOH:O	2.10	0.69
1:A:269:ASP:O	8:A:1002:HOH:O	2.11	0.68
1:A:608:ASP:O	8:A:1003:HOH:O	2.12	0.68
1:A:402:GLU:HG2	8:A:1012:HOH:O	1.99	0.63
1:A:344:CYS:O	1:A:345:HIS:C	2.50	0.55
1:A:132:LYS:HE3	1:A:142:CYS:HB3	1.89	0.55
1:A:701:ASP:OD1	1:A:704:ARG:NH2	2.41	0.54
1:A:499:ASP:N	1:A:500:PRO:CD	2.73	0.51
1:A:589:LYS:N	1:A:590:PRO:HD2	2.28	0.48
1:A:450:LEU:N	1:A:451:PRO:CD	2.78	0.46
1:A:177:ARG:HB3	1:A:178:PRO:HD3	2.00	0.44
1:A:582:LYS:HB2	1:A:583:PRO:HD3	2.00	0.44
1:A:397:ASN:O	8:A:1004:HOH:O	2.21	0.43
2:B:559:ASP:OD1	2:B:559:ASP:C	2.61	0.43
1:A:582:LYS:N	1:A:583:PRO:CD	2.82	0.42
1:A:27:ARG:HH11	6:A:901:NAG:H61	1.71	0.42
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.02	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	705/891 (79%)	697 (99%)	8 (1%)	0	100	100
2	B	186/315 (59%)	181 (97%)	5 (3%)	0	100	100
All	All	891/1206 (74%)	878 (98%)	13 (2%)	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	536/769 (70%)	534 (100%)	2 (0%)	84	92
2	B	104/270 (38%)	103 (99%)	1 (1%)	68	84
All	All	640/1039 (62%)	637 (100%)	3 (0%)	78	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	A	552	LYS
2	B	517	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	39	ASN
1	A	97	GLN
1	A	239	GLN
1	A	374	HIS
1	A	445	ASN
1	A	505	HIS
1	A	599	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 ⓘ

18 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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	1.15	2 (14%)	17,19,21	1.15	2 (11%)
3	NAG	C	2	3	14,14,15	1.05	2 (14%)	17,19,21	1.01	2 (11%)
3	FUC	C	3	3	10,10,11	1.02	0	14,14,16	0.50	0
4	NAG	D	1	1,4	14,14,15	1.13	1 (7%)	17,19,21	1.10	1 (5%)
4	NAG	D	2	4	14,14,15	1.19	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	E	1	1,4	14,14,15	1.15	1 (7%)	17,19,21	1.11	1 (5%)
4	NAG	E	2	4	14,14,15	1.17	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.93	2 (14%)	17,19,21	1.15	1 (5%)
3	NAG	F	2	3	14,14,15	1.06	2 (14%)	17,19,21	0.94	1 (5%)
3	FUC	F	3	3	10,10,11	1.05	0	14,14,16	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	1	1,5	14,14,15	1.24	1 (7%)	17,19,21	1.17	1 (5%)
5	NAG	G	2	5	14,14,15	0.43	0	17,19,21	0.76	0
5	BMA	G	3	5	11,11,12	1.14	1 (9%)	15,15,17	0.65	0
4	NAG	H	1	1,4	14,14,15	0.42	0	17,19,21	0.72	0
4	NAG	H	2	4	14,14,15	1.01	1 (7%)	17,19,21	1.06	2 (11%)
5	NAG	I	1	2,5	14,14,15	1.12	1 (7%)	17,19,21	1.17	1 (5%)
5	NAG	I	2	5	14,14,15	1.06	1 (7%)	17,19,21	1.18	3 (17%)
5	BMA	I	3	5	11,11,12	1.01	0	15,15,17	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	FUC	C	3	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C1-C2	3.54	1.57	1.52
4	E	1	NAG	C1-C2	3.42	1.57	1.52
4	E	2	NAG	C1-C2	3.41	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	NAG	C1-C2	3.27	1.56	1.52
3	C	1	NAG	C1-C2	3.22	1.56	1.52
4	D	1	NAG	C1-C2	3.16	1.56	1.52
5	I	1	NAG	C1-C2	3.11	1.56	1.52
5	I	2	NAG	C1-C2	3.00	1.56	1.52
4	H	2	NAG	C1-C2	2.70	1.56	1.52
3	F	2	NAG	C1-C2	2.59	1.55	1.52
5	G	3	BMA	O5-C5	2.37	1.48	1.43
3	C	2	NAG	O5-C5	2.30	1.47	1.43
3	C	1	NAG	O5-C5	2.15	1.47	1.43
3	F	1	NAG	C1-C2	2.15	1.55	1.52
3	F	1	NAG	O5-C5	2.08	1.47	1.43
3	F	2	NAG	O5-C5	2.07	1.47	1.43
3	C	2	NAG	C1-C2	2.02	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	-3.36	118.40	122.90
3	C	1	NAG	C2-N2-C7	-2.91	119.00	122.90
4	E	1	NAG	C8-C7-N2	2.71	120.62	116.12
5	I	1	NAG	C8-C7-N2	2.69	120.58	116.12
4	H	2	NAG	C8-C7-N2	2.53	120.31	116.12
4	D	1	NAG	C8-C7-N2	2.42	120.13	116.12
5	G	1	NAG	C8-C7-N2	2.39	120.08	116.12
4	D	2	NAG	C8-C7-N2	2.28	119.90	116.12
4	E	2	NAG	C8-C7-N2	2.26	119.87	116.12
5	I	2	NAG	C1-O5-C5	2.25	115.20	112.19
3	F	2	NAG	C8-C7-N2	2.25	119.84	116.12
5	I	2	NAG	C8-C7-N2	2.16	119.69	116.12
4	H	2	NAG	C2-N2-C7	-2.16	120.01	122.90
3	C	1	NAG	C8-C7-N2	2.12	119.64	116.12
5	I	2	NAG	C2-N2-C7	-2.07	120.13	122.90
3	C	2	NAG	C2-N2-C7	-2.06	120.14	122.90
3	C	2	NAG	C8-C7-N2	2.03	119.49	116.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2

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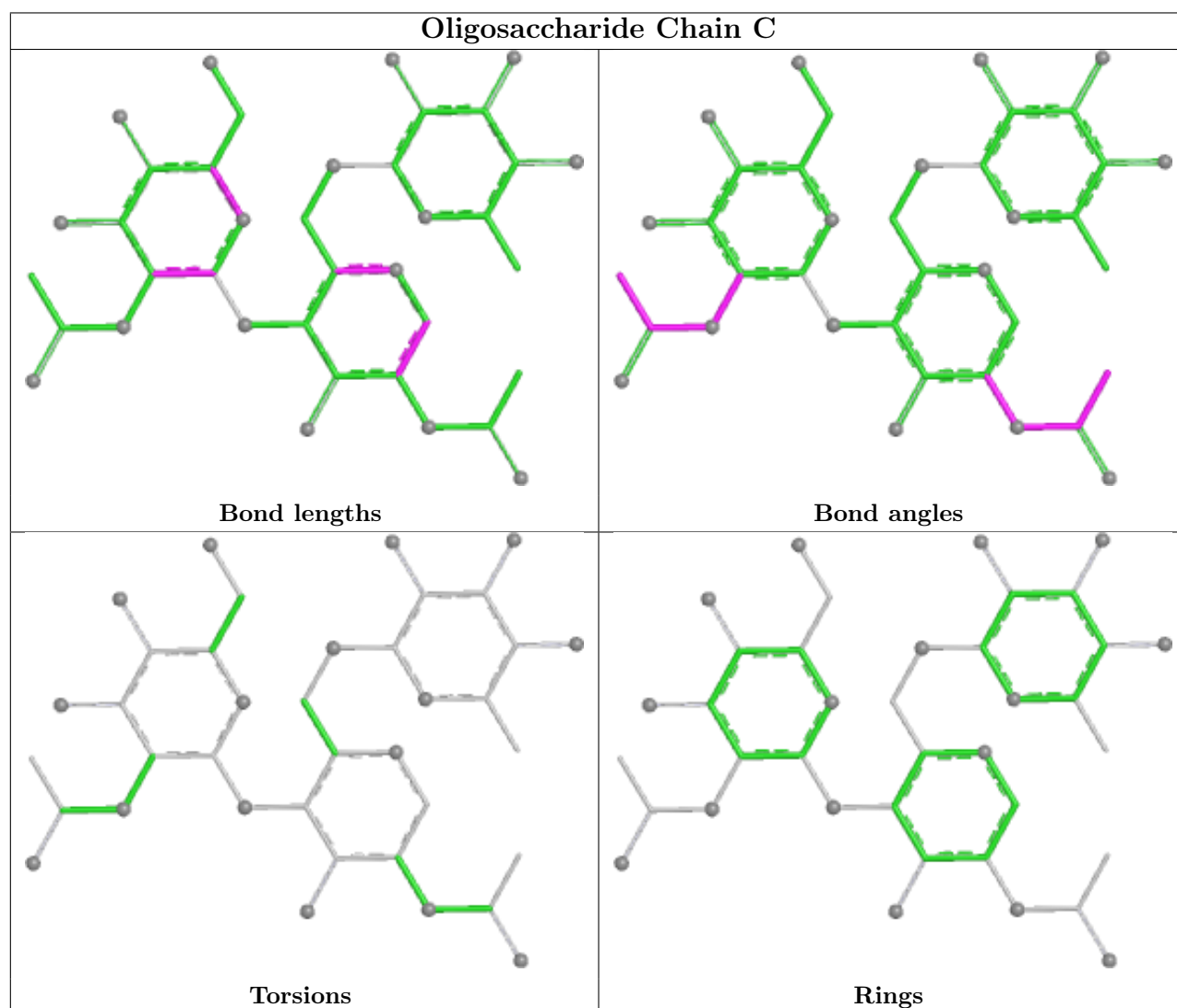
Continued from previous page...

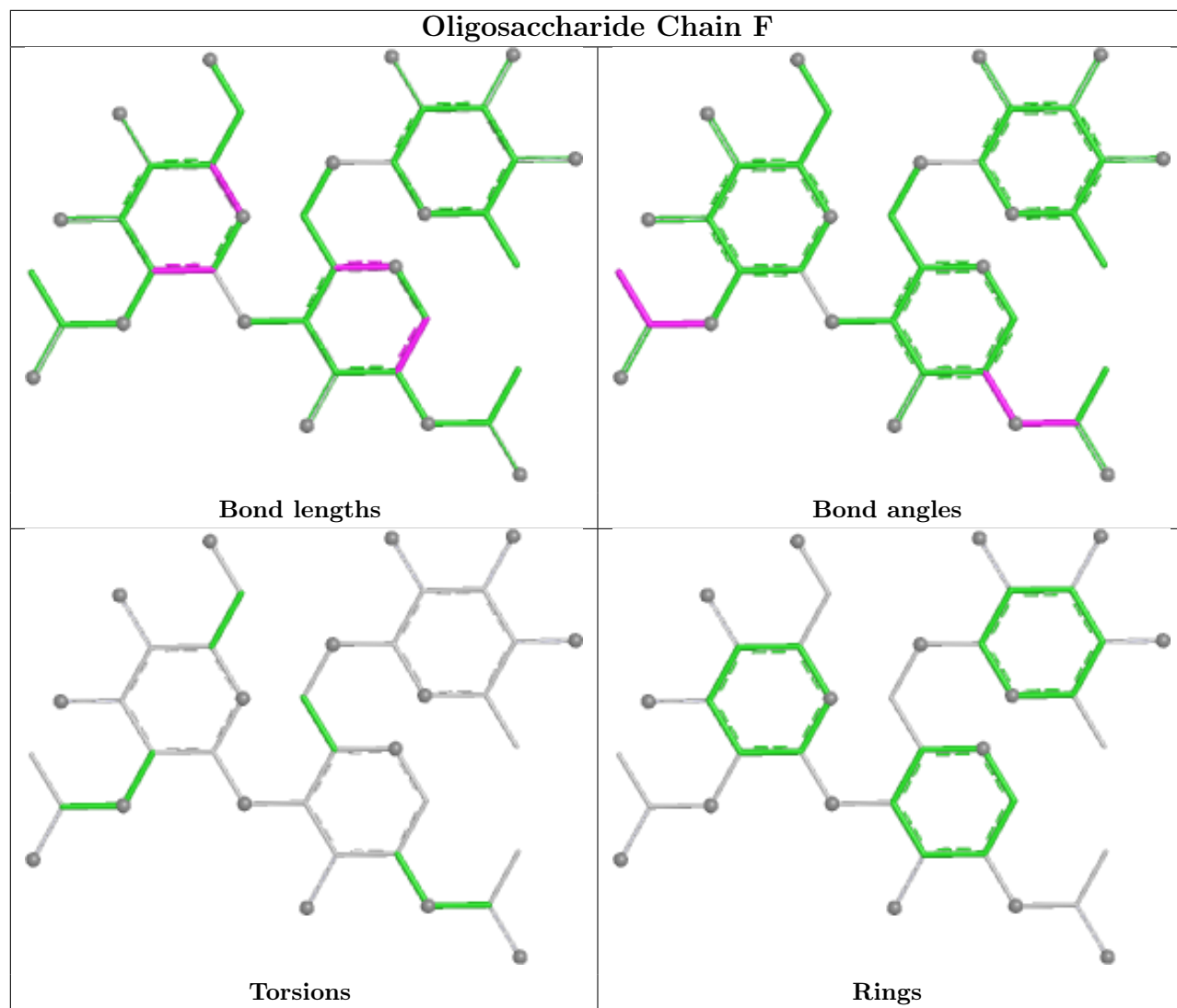
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6

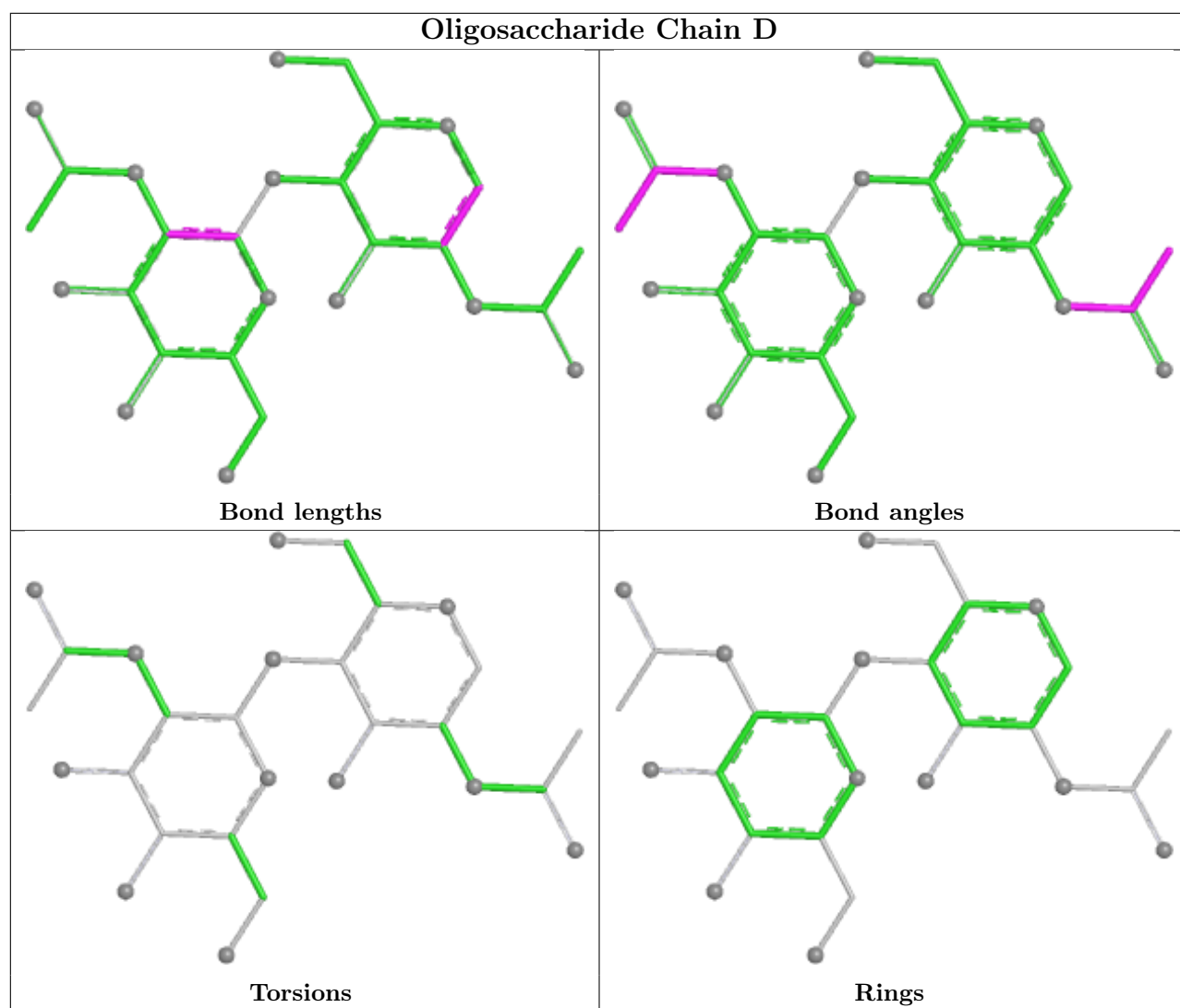
There are no ring outliers.

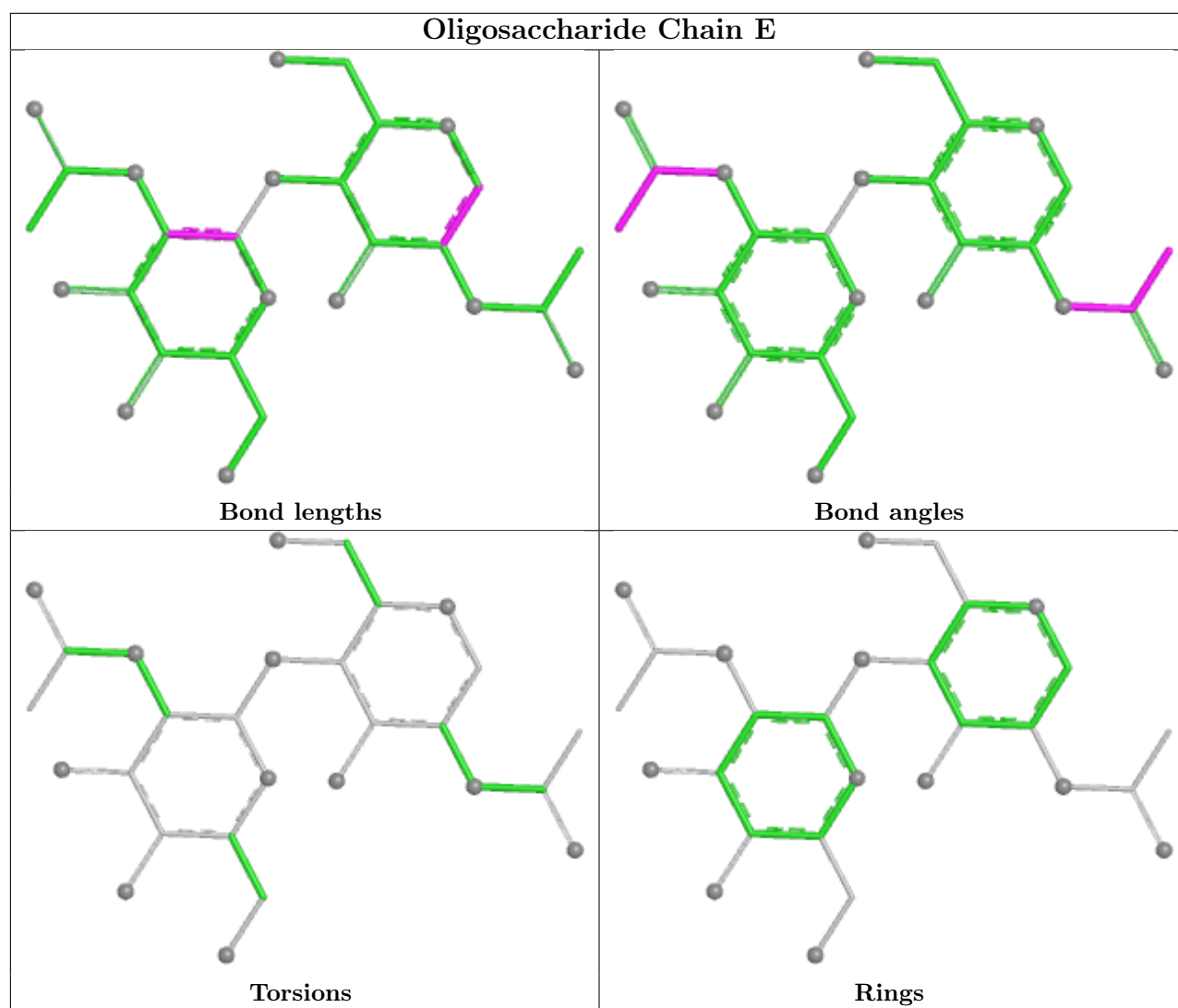
No monomer is involved in short contacts.

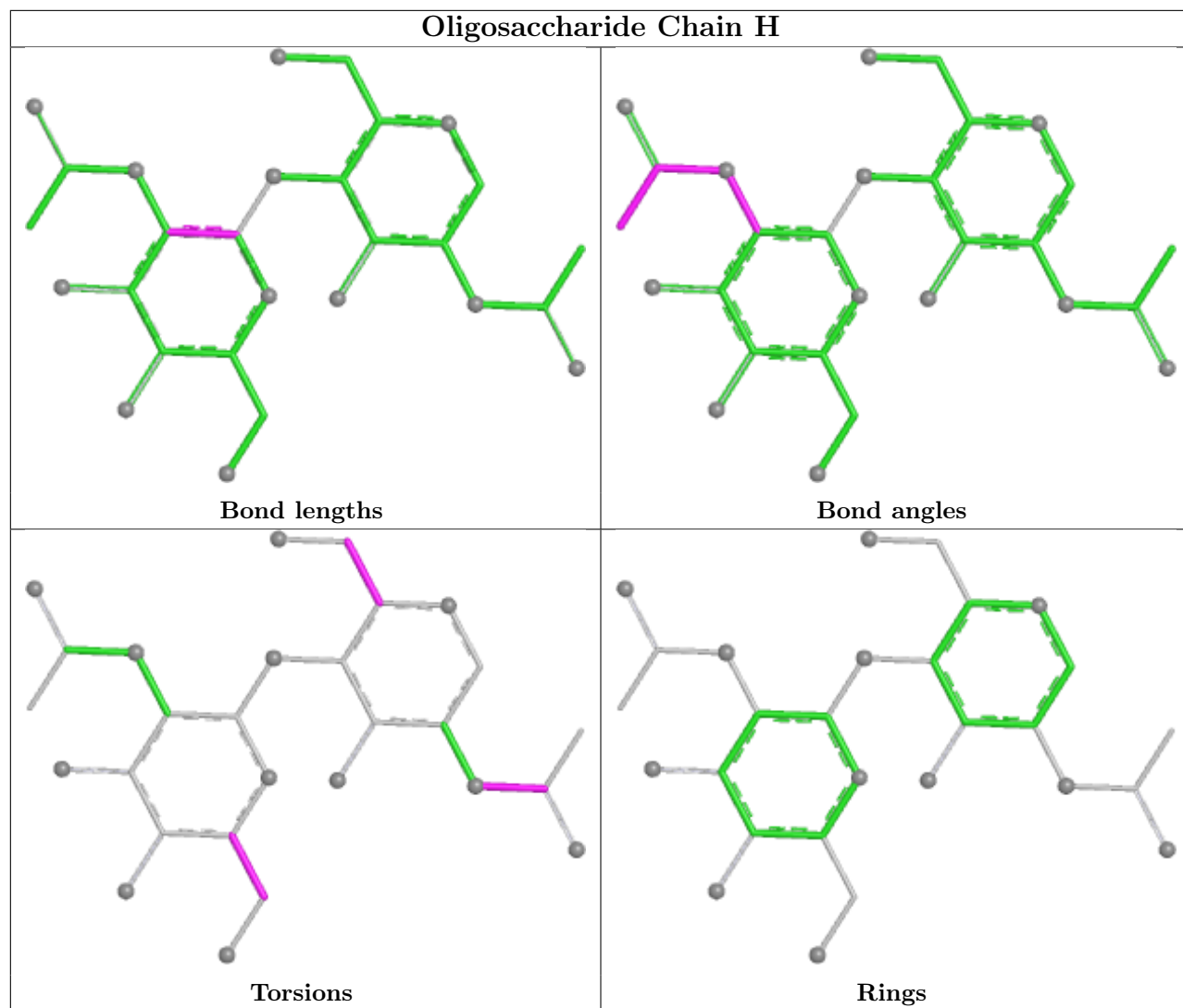
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

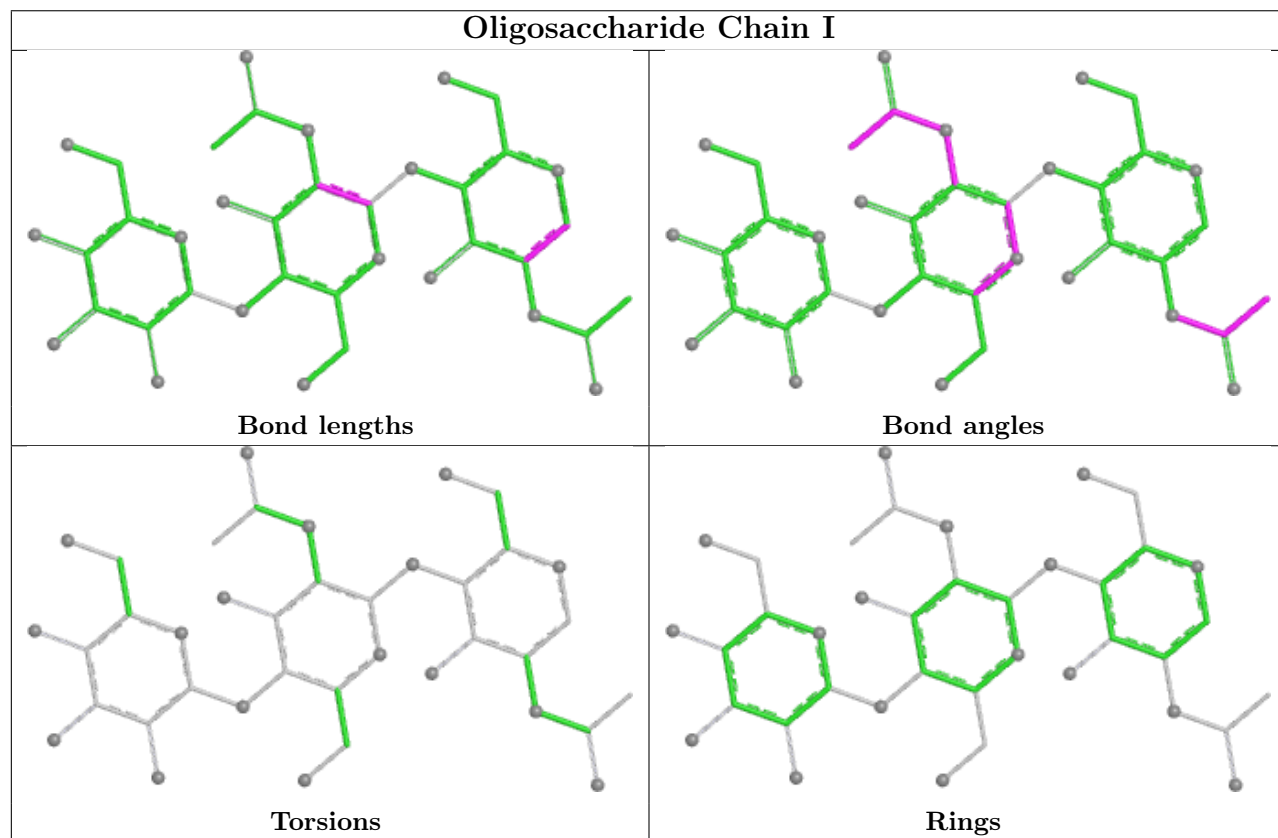
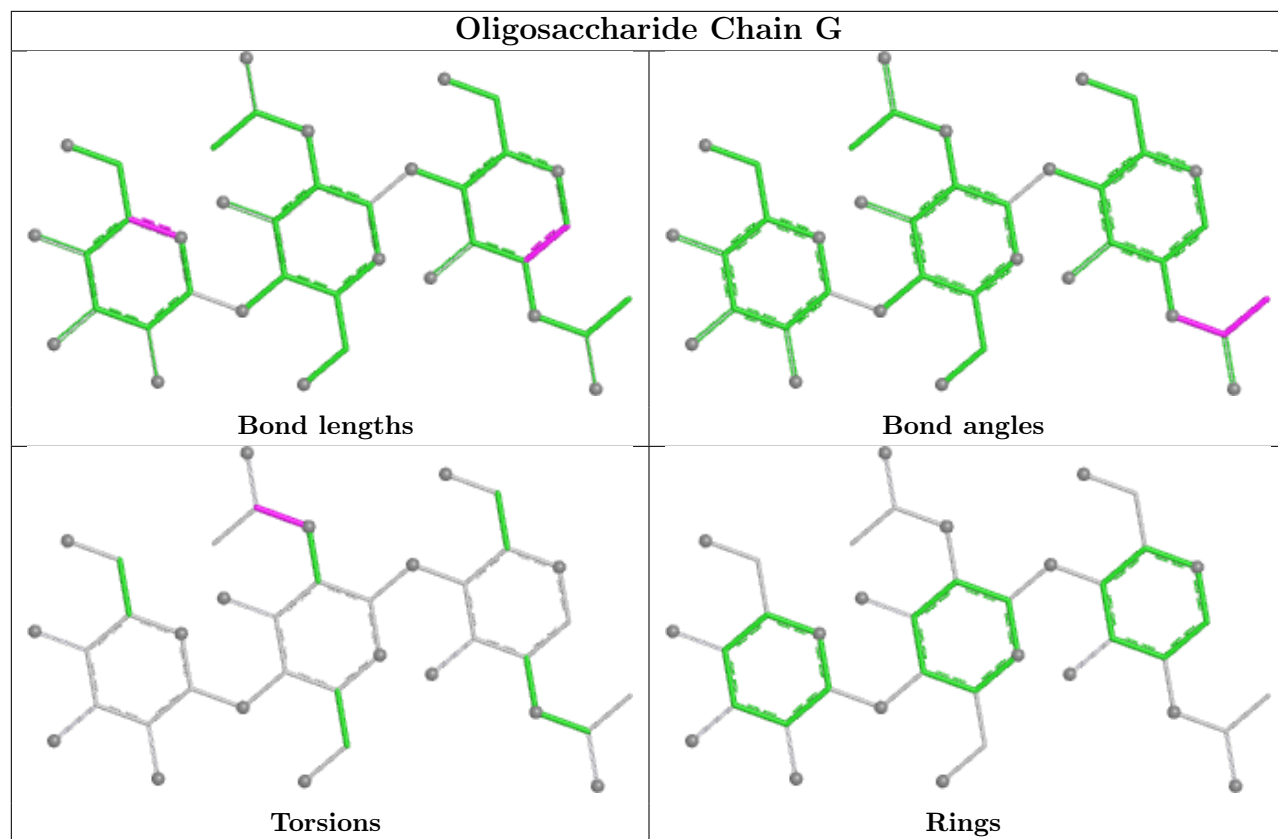












5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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
6	NAG	A	902	1	14,14,15	1.57	2 (14%)	17,19,21	0.83	0
6	NAG	B	701	2	14,14,15	1.18	1 (7%)	17,19,21	1.12	1 (5%)
6	NAG	A	901	1	14,14,15	1.24	1 (7%)	17,19,21	1.07	1 (5%)
6	NAG	A	903	1	14,14,15	1.23	1 (7%)	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
6	NAG	B	701	2	-	0/6/23/26	0/1/1/1
6	NAG	A	901	1	-	0/6/23/26	0/1/1/1
6	NAG	A	903	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	902	NAG	C1-C2	4.83	1.58	1.52
6	A	903	NAG	C1-C2	3.81	1.57	1.52
6	A	901	NAG	C1-C2	3.67	1.57	1.52
6	B	701	NAG	C1-C2	3.29	1.56	1.52
6	A	902	NAG	O5-C5	2.08	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	701	NAG	C8-C7-N2	2.63	120.48	116.12
6	A	901	NAG	C8-C7-N2	2.47	120.22	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	903	NAG	C8-C7-N2	2.36	120.03	116.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	NAG	5	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.

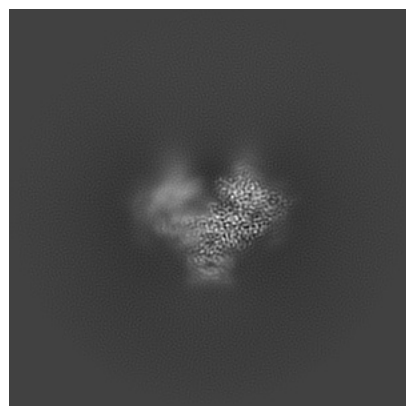
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46691. These allow visual inspection of the internal detail of the map and identification of artifacts.

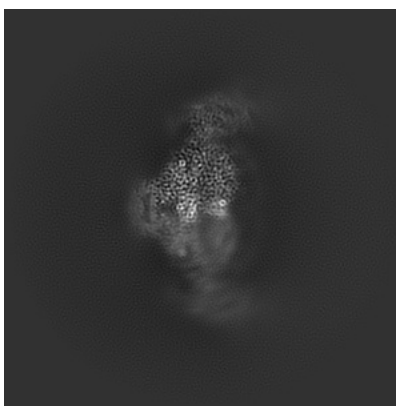
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

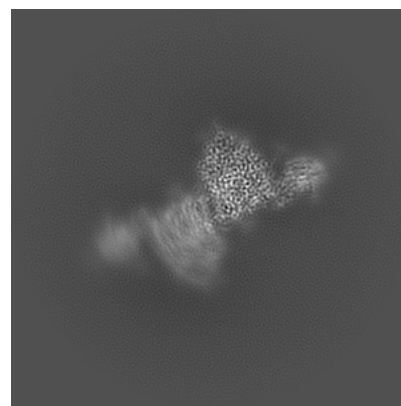
6.1.1 Primary map



X

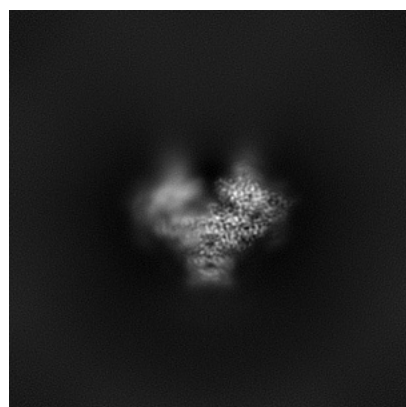


Y

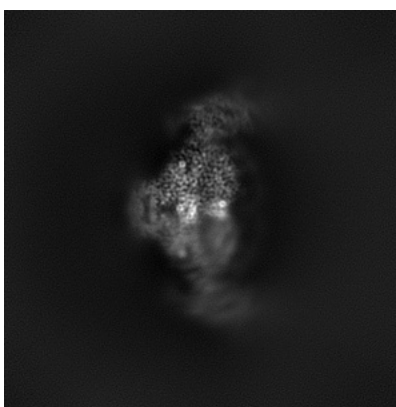


Z

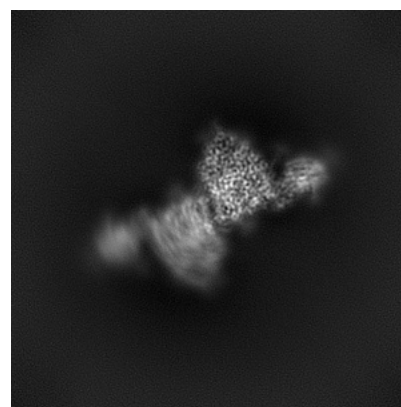
6.1.2 Raw map



X



Y

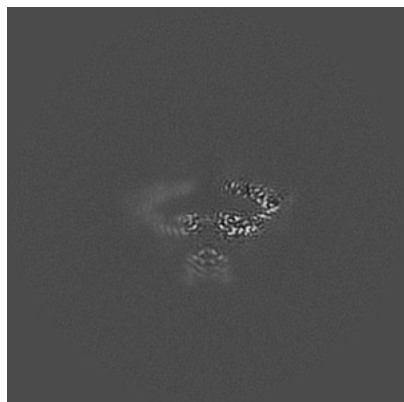


Z

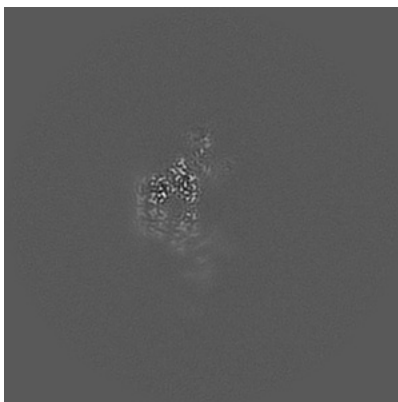
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

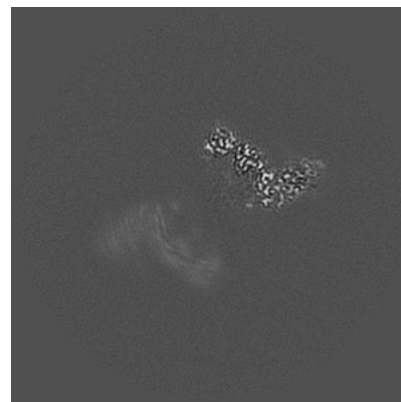
6.2.1 Primary map



X Index: 160



Y Index: 160

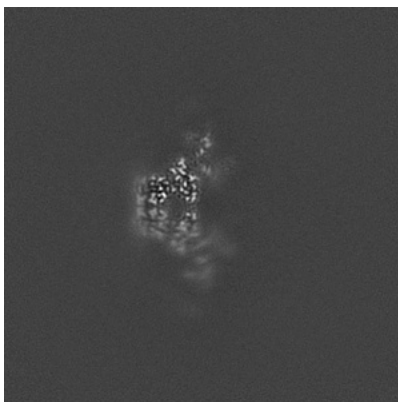


Z Index: 160

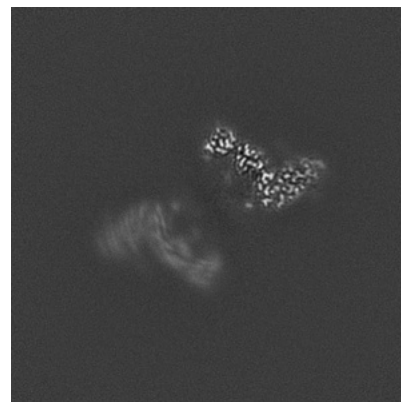
6.2.2 Raw map



X Index: 160



Y Index: 160

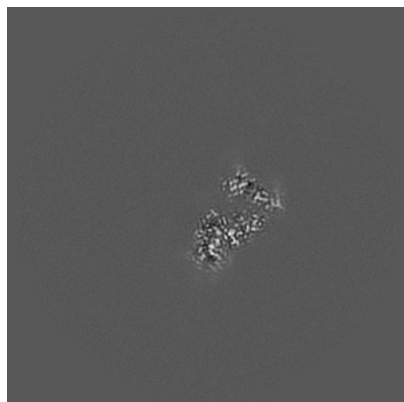


Z Index: 160

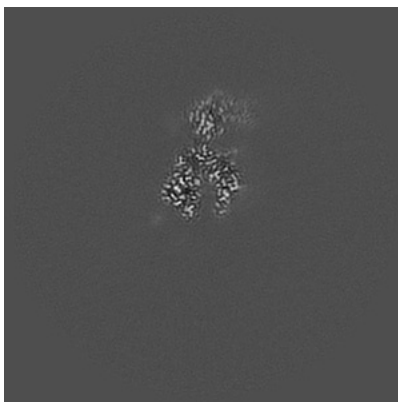
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

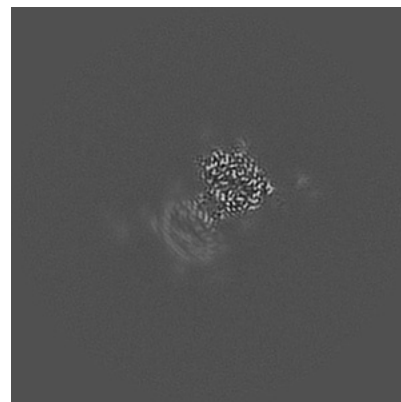
6.3.1 Primary map



X Index: 176

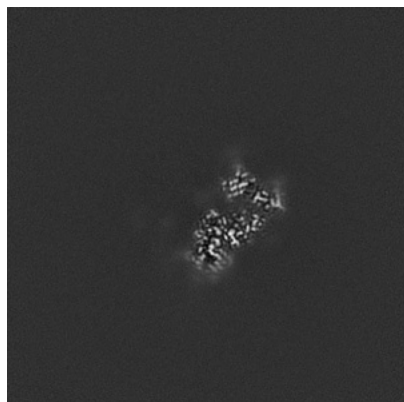


Y Index: 184

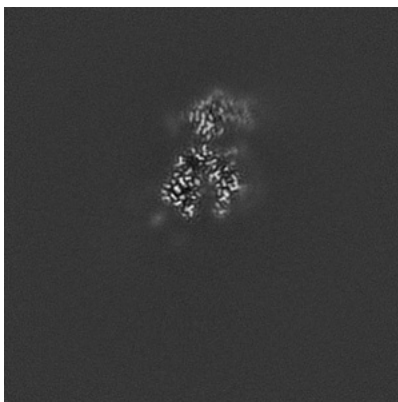


Z Index: 143

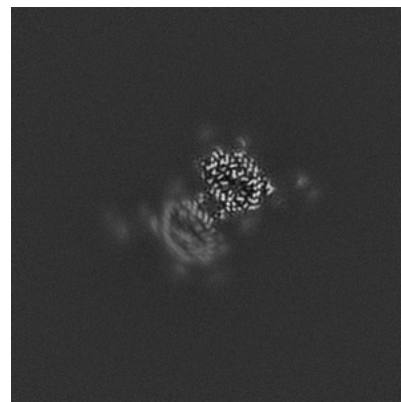
6.3.2 Raw map



X Index: 176



Y Index: 184

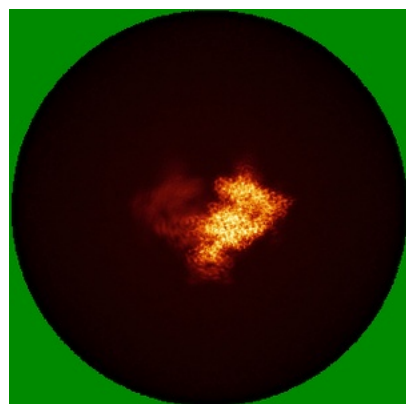


Z Index: 143

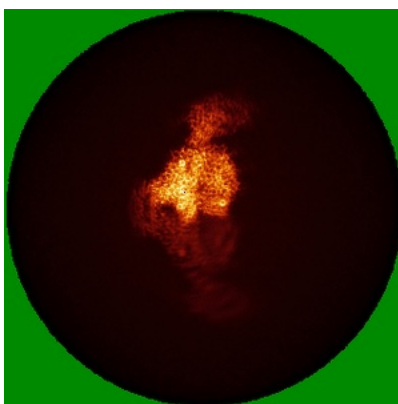
The images above show the largest variance slices of the map in three orthogonal directions.

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

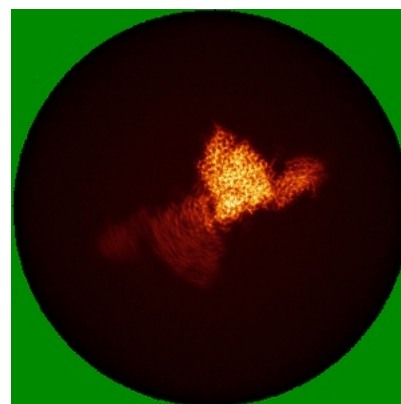
6.4.1 Primary map



X

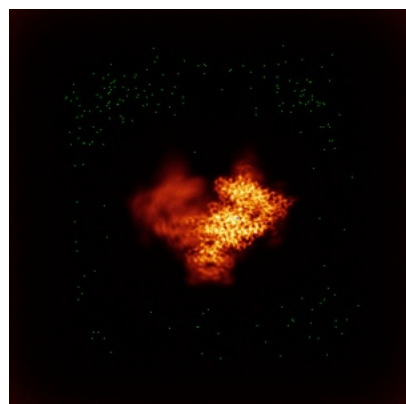


Y

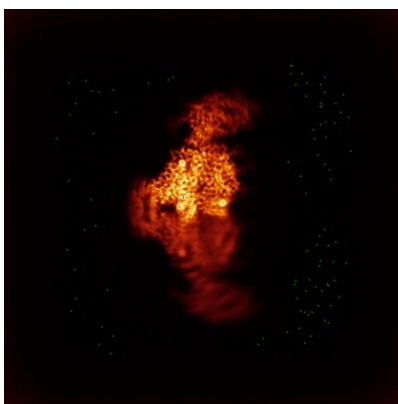


Z

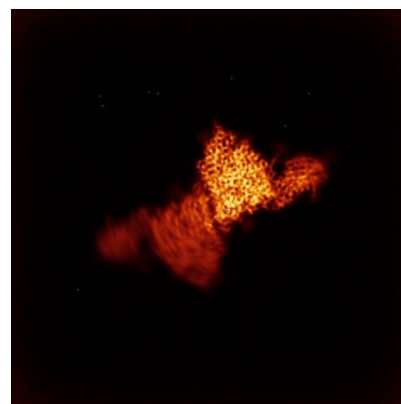
6.4.2 Raw map



X



Y

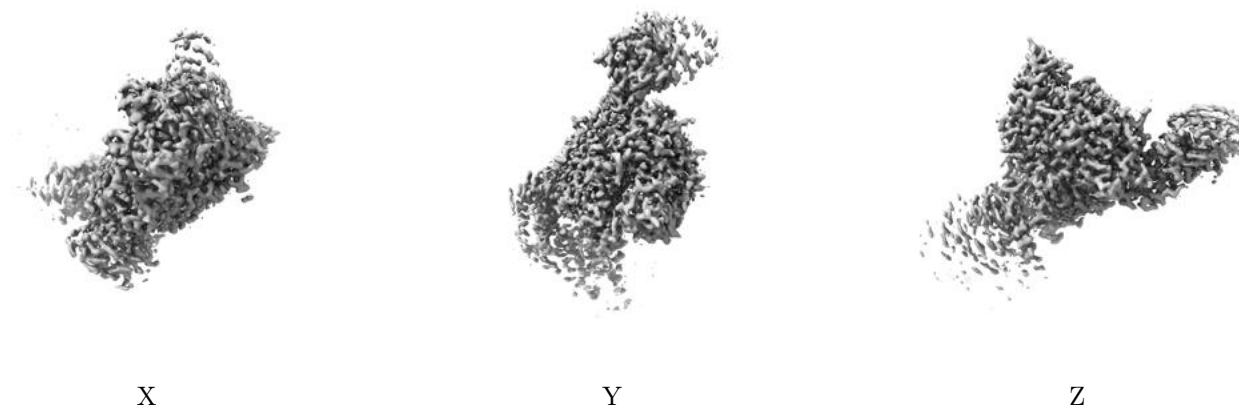


Z

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 0.4. 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.

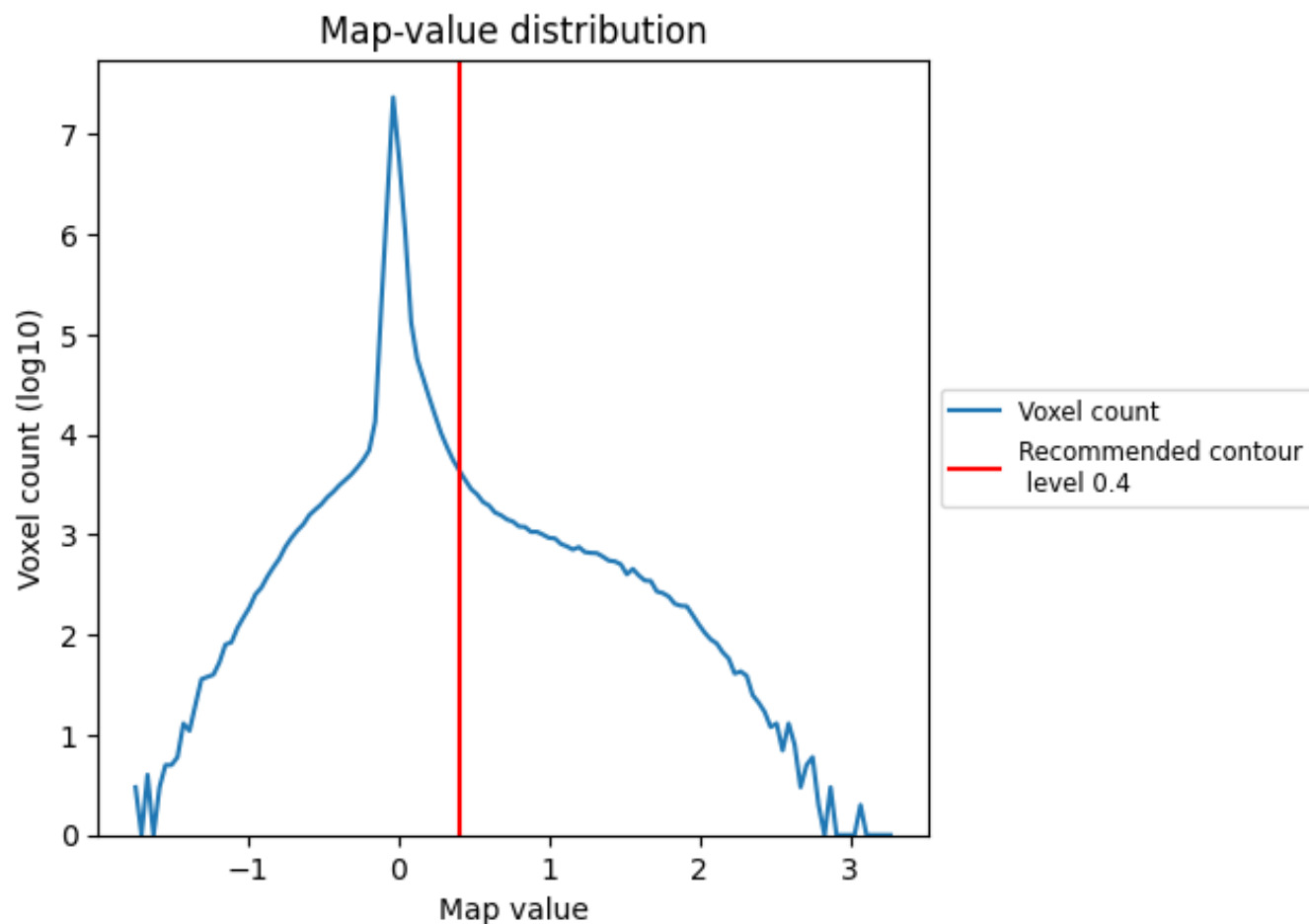
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

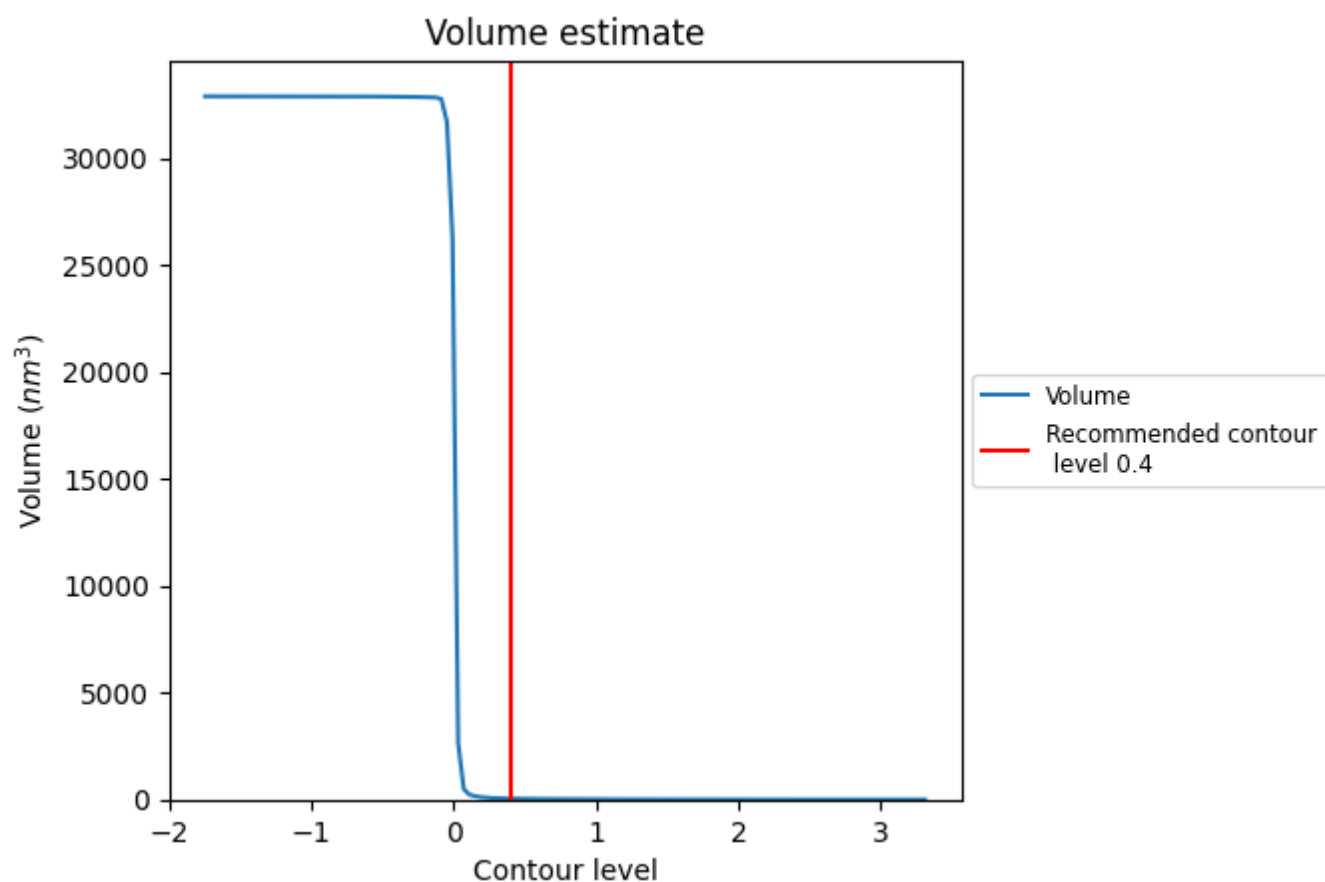
This section contains the results of statistical analysis of the map.

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.

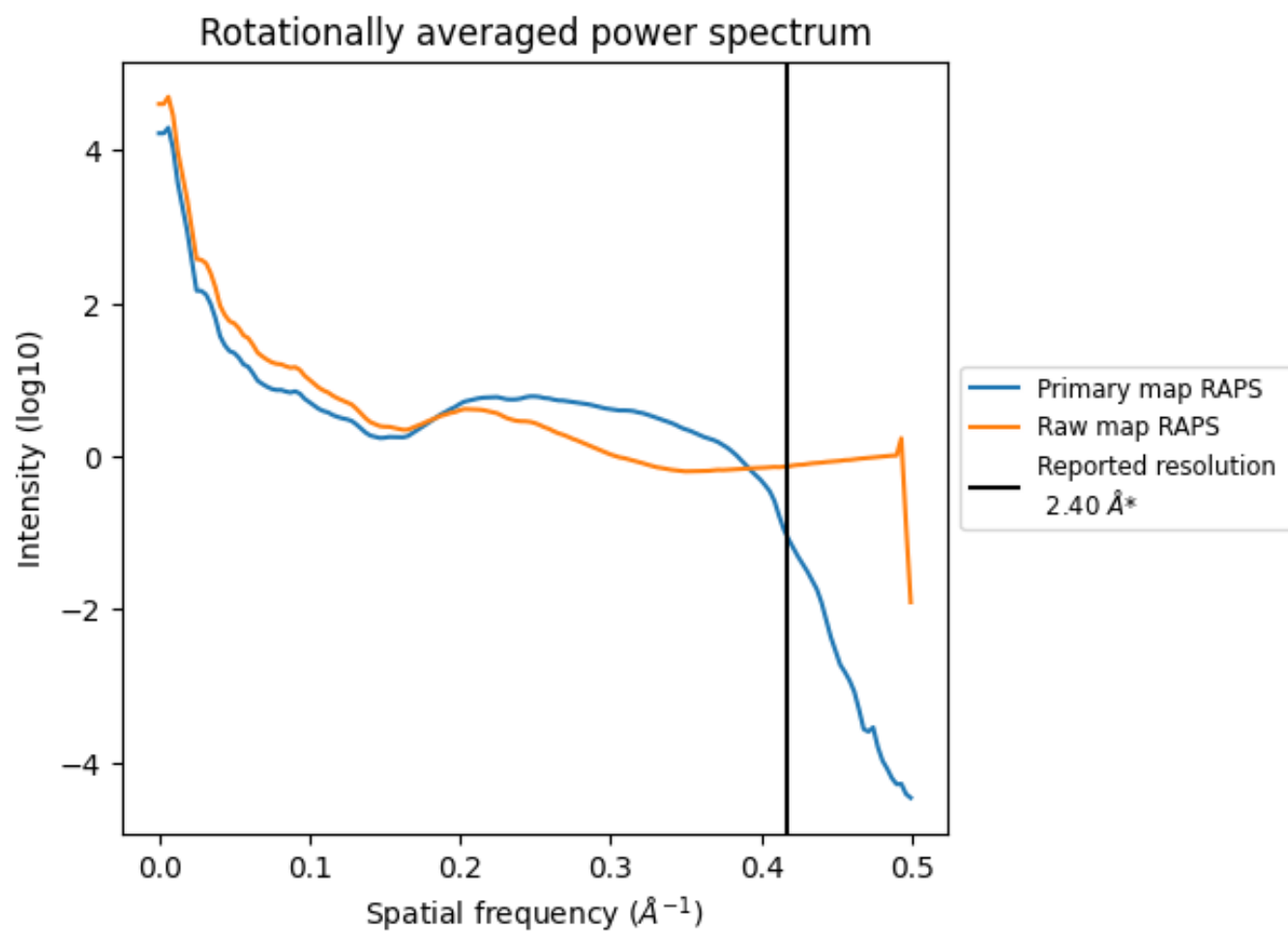
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 43 nm³; this corresponds to an approximate mass of 39 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 ⓘ

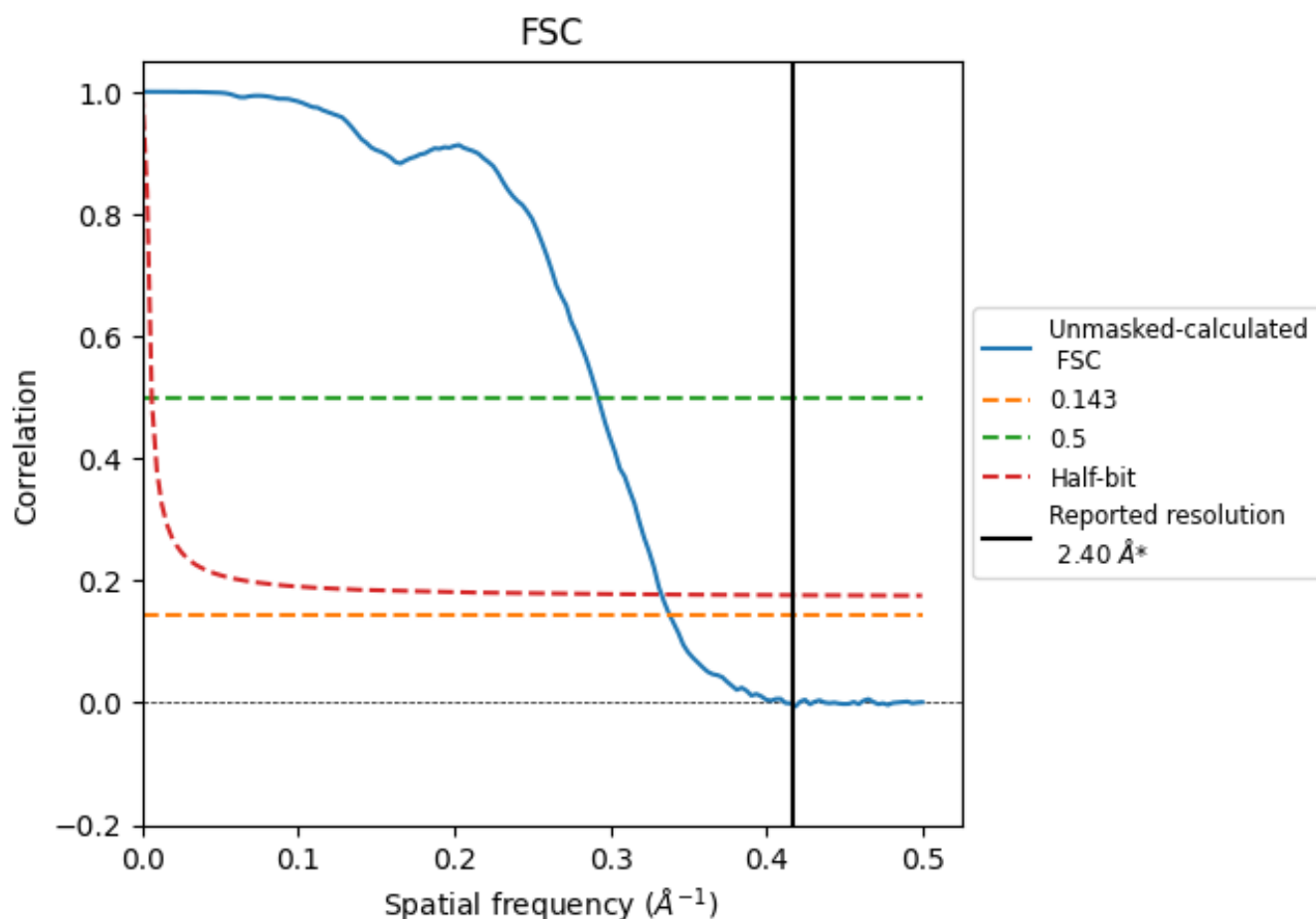


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.96	3.43	3.01

*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 2.96 differs from the reported value 2.4 by more than 10 %

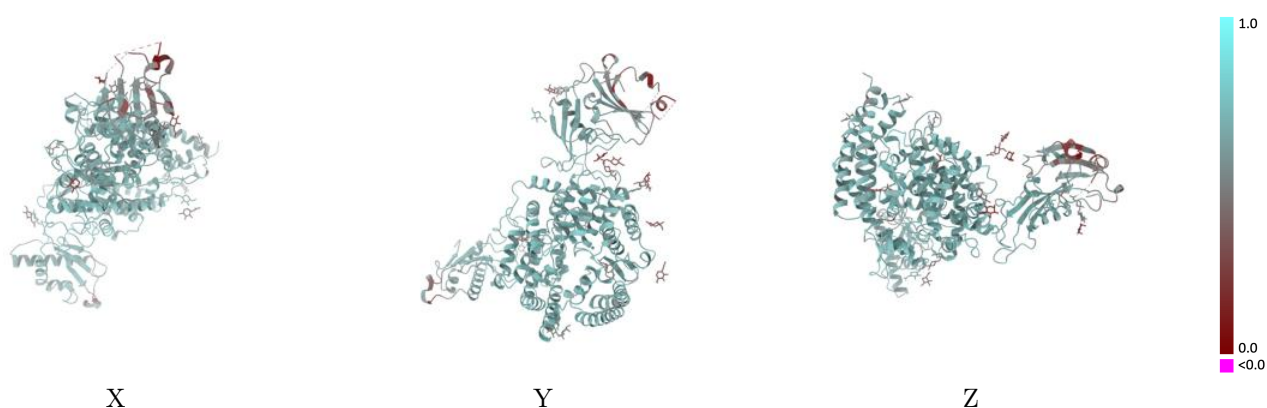
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-46691 and PDB model 9DAK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)

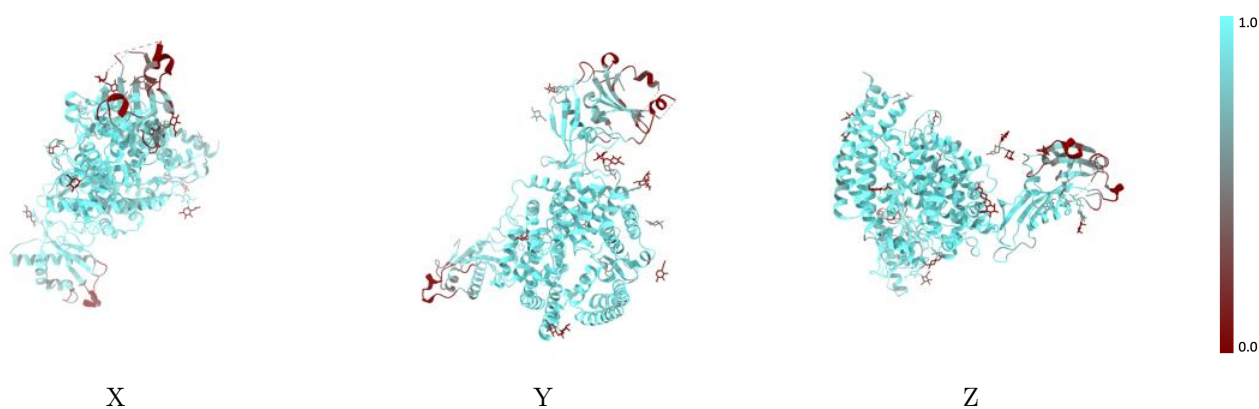
This section was not generated.

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



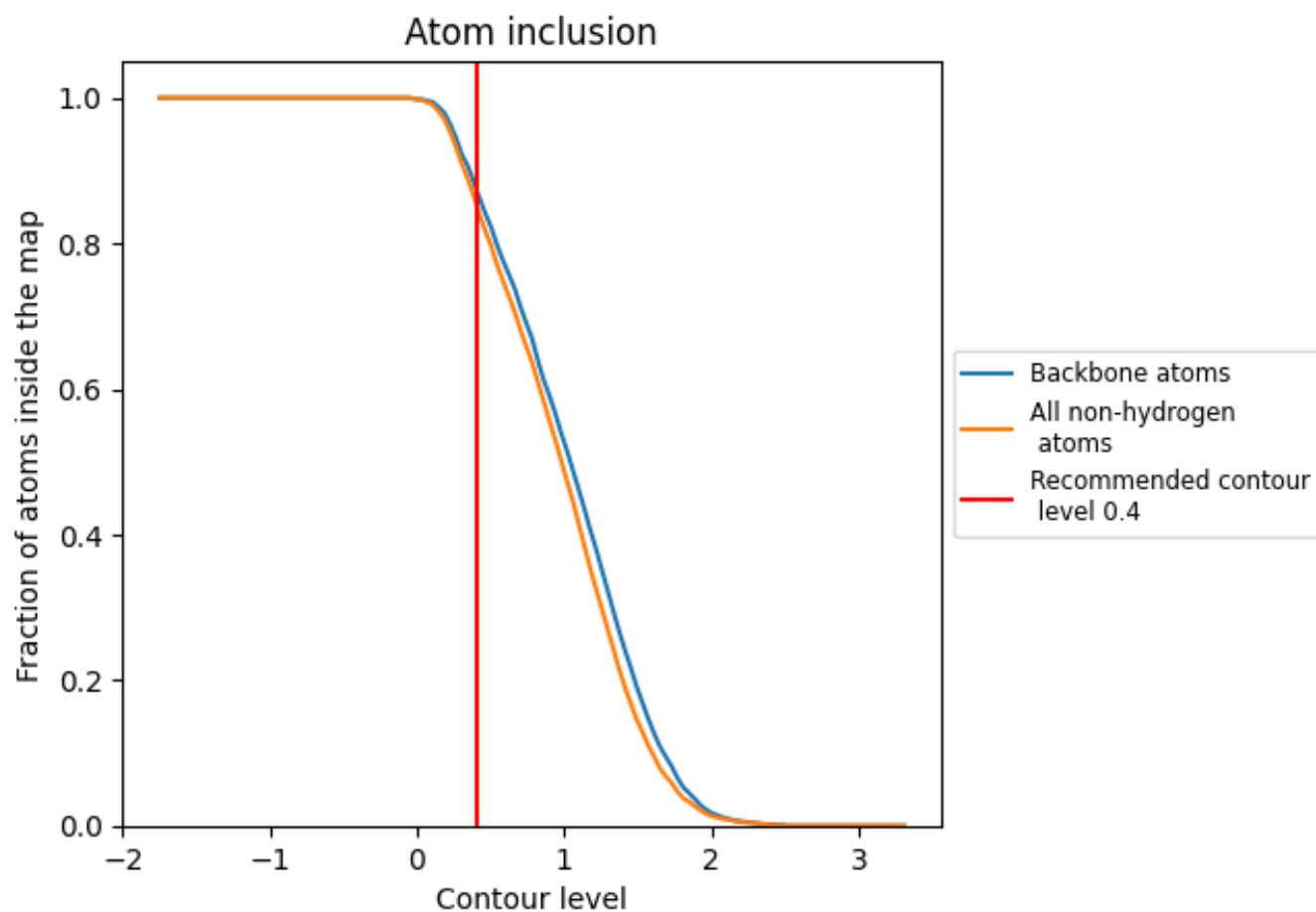
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.6320
A	0.9130	0.6560
B	0.7020	0.5660
C	0.3680	0.5270
D	0.5000	0.5070
E	0.4640	0.5320
F	0.1580	0.3060
G	0.2560	0.3970
H	0.6430	0.5160
I	0.4870	0.4250

1.0

0.0

<0.0