



Full wwPDB EM Validation Report ⓘ

Jun 30, 2026 – 08:26 PM EDT

PDB ID : 9OW3 / pdb_00009ow3
EMDB ID : EMD-70927
Title : Hedgehog coronavirus ErinCoV-12-19 spike receptor binding domain in complex with hedgehog APN (locally refined)
Authors : Jin, M.; Rini, J.M.
Deposited on : 2025-06-02
Resolution : 2.01 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:

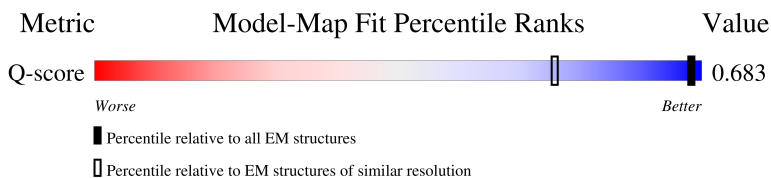
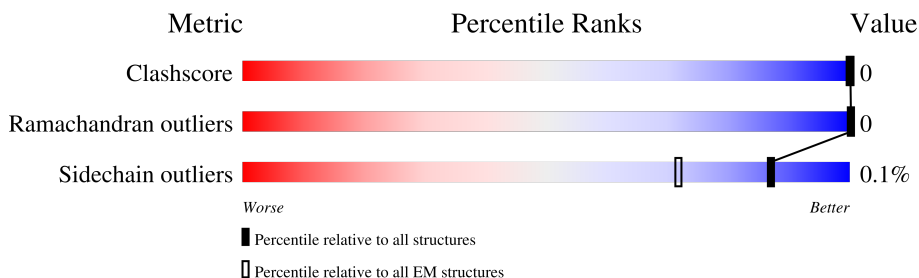
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.01 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	1691 (1.52 - 2.51)

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	900	99%
2	B	4	25% (red), 75% (green), 25% (orange)
3	C	209	10% (red), 100% (green)
4	D	2	100% (yellow)

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 100%
4	G	2	 50% 100%
5	H	3	 100%
6	I	3	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18303 atoms, of which 8946 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 Aminopeptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	900	14307	4629	7051	1234	1371	22	0	0

- Molecule 2 is a protein called Amastatin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	B	4	70	21	37	4	8	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	208	3179	1024	1564	267	312	12	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	372	GLU	ASP	conflict	UNP U5LMM7
C	407	GLU	GLN	conflict	UNP U5LMM7
C	412	ILE	VAL	conflict	UNP U5LMM7
C	458	LYS	ASN	conflict	UNP U5LMM7
C	474	GLY	ALA	conflict	UNP U5LMM7
C	485	SER	ASN	conflict	UNP U5LMM7
C	497	THR	VAL	conflict	UNP U5LMM7
C	512	VAL	ILE	conflict	UNP U5LMM7
C	513	VAL	ALA	conflict	UNP U5LMM7
C	519	ILE	LEU	conflict	UNP U5LMM7
C	536	THR	ASN	conflict	UNP U5LMM7
C	545	ASN	LYS	conflict	UNP U5LMM7
C	548	VAL	THR	conflict	UNP U5LMM7
C	550	ASN	GLU	conflict	UNP U5LMM7
C	?	-	GLY	deletion	UNP U5LMM7

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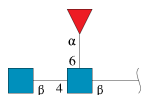
Chain	Residue	Modelled	Actual	Comment	Reference
C	552	ILE	VAL	conflict	UNP U5LMM7
C	561	ASN	LYS	conflict	UNP U5LMM7
C	563	ASN	ASP	conflict	UNP U5LMM7

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



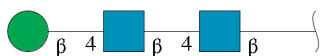
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	D	2	55	16	27	2	10	0	0
4	E	2	55	16	27	2	10	0	0
4	F	2	55	16	27	2	10	0	0
4	G	2	55	16	27	2	10	0	0

- 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.



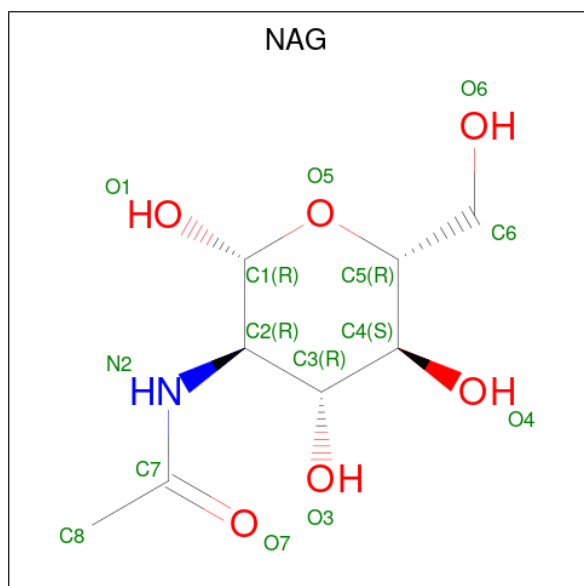
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
5	H	3	75	22	37	2	14	0	0

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



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	I	3	76	22	37	2	15	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
7	A	1	28	8	14	1	5	0
7	A	1	28	8	14	1	5	0
7	A	1	28	8	14	1	5	0
7	A	1	28	8	14	1	5	0
7	C	1	28	8	14	1	5	0
7	C	1	28	8	14	1	5	0
7	C	1	28	8	14	1	5	0
7	C	1	28	8	14	1	5	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

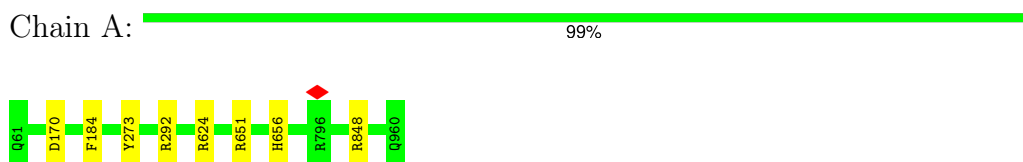
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	140	Total 140	O 140	0
9	C	11	Total 11	O 11	0

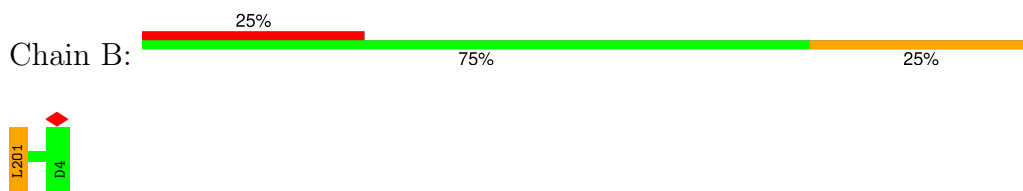
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

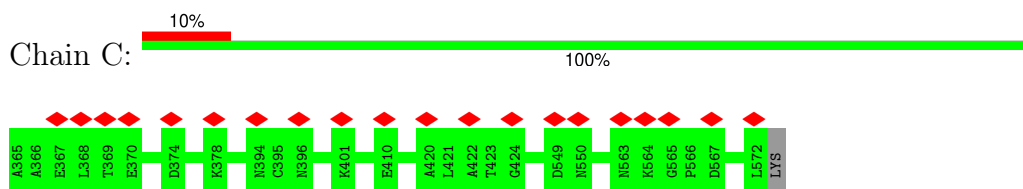
- Molecule 1: Aminopeptidase



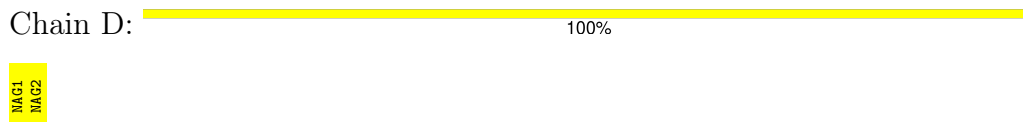
- Molecule 2: Amastatin



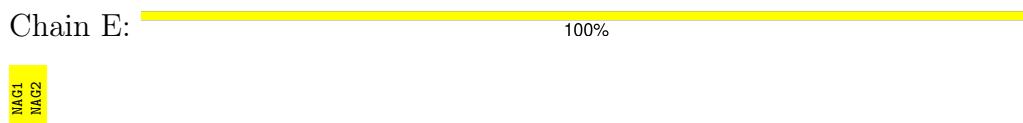
- Molecule 3: Spike glycoprotein



- 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

Chain F:  100%

NAG1
NAG2

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

Chain G:  50%
100%


NAG1
NAG2

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

Chain H:  100%

NAG1
NAG2
FUC3

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

Chain I:  100%

NAG1
NAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1578752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	4.301	Depositor
Minimum map value	-5.407	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	374.784, 374.784, 374.784	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	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: FUC, BMA, L2O, ZN, 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	0.71	0/7442	1.24	7/10140 (0.1%)
2	B	0.84	0/22	1.44	0/28
3	C	0.72	0/1652	1.20	0/2251
All	All	0.72	0/9116	1.23	7/12419 (0.1%)

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
2	B	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	624	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	656	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	A	848	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	170	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	184	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	292	ARG	NE-CZ-NH2	5.03	123.72	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	L2O	Mainchain,Peptide

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	7256	7051	7046	0	0
2	B	33	37	29	0	0
3	C	1615	1564	1561	0	0
4	D	28	27	25	0	0
4	E	28	27	25	0	0
4	F	28	27	25	0	0
4	G	28	27	25	0	0
5	H	38	37	34	0	0
6	I	39	37	34	0	0
7	A	56	56	52	0	0
7	C	56	56	52	0	0
8	A	1	0	0	0	0
9	A	140	0	0	0	0
9	C	11	0	0	0	0
All	All	9357	8946	8908	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	898/900 (100%)	874 (97%)	24 (3%)	0	100	100
2	B	2/4 (50%)	2 (100%)	0	0	100	100
3	C	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
All	All	1106/1113 (99%)	1072 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	797/797 (100%)	796 (100%)	1 (0%)	88	92
2	B	3/3 (100%)	3 (100%)	0	100	100
3	C	179/180 (99%)	179 (100%)	0	100	100
All	All	979/980 (100%)	978 (100%)	1 (0%)	87	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	TYR

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	160	ASN
1	A	202	GLN
1	A	513	GLN
1	A	517	ASN
1	A	591	HIS
3	C	495	GLN
3	C	561	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	L2O	B	1	8,2	7,9,10	1.00	1 (14%)	6,11,13	2.29	3 (50%)

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	L2O	B	1	8,2	-	6/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	L2O	C2-CA	2.05	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	L2O	O1-C6-CA	3.84	113.78	107.31
2	B	1	L2O	O1-C6-C	-3.42	102.71	110.48
2	B	1	L2O	C3-C2-CA	-2.12	111.20	115.76

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	L2O	C-C6-CA-N
2	B	1	L2O	CA-C2-C3-C4
2	B	1	L2O	CA-C2-C3-C5
2	B	1	L2O	O1-C6-CA-C2
2	B	1	L2O	C-C6-CA-C2
2	B	1	L2O	O-C-C6-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

14 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	D	1	1,4	14,14,15	1.23	1 (7%)	17,19,21	1.27	3 (17%)
4	NAG	D	2	4	14,14,15	1.26	2 (14%)	17,19,21	1.11	1 (5%)
4	NAG	E	1	1,4	14,14,15	1.15	1 (7%)	17,19,21	0.63	0
4	NAG	E	2	4	14,14,15	1.28	2 (14%)	17,19,21	0.84	1 (5%)
4	NAG	F	1	1,4	14,14,15	1.18	1 (7%)	17,19,21	1.01	2 (11%)
4	NAG	F	2	4	14,14,15	1.25	2 (14%)	17,19,21	0.76	0
4	NAG	G	1	1,4	14,14,15	1.26	2 (14%)	17,19,21	0.74	0
4	NAG	G	2	4	14,14,15	1.26	2 (14%)	17,19,21	0.81	1 (5%)
5	NAG	H	1	1,5	14,14,15	0.44	0	17,19,21	0.73	0
5	NAG	H	2	5	14,14,15	0.41	0	17,19,21	0.47	0
5	FUC	H	3	5	10,10,11	0.46	0	14,14,16	0.30	0
6	NAG	I	1	1,6	14,14,15	1.17	1 (7%)	17,19,21	0.90	1 (5%)
6	NAG	I	2	6	14,14,15	1.29	2 (14%)	17,19,21	0.73	0
6	BMA	I	3	6	11,11,12	1.38	2 (18%)	15,15,17	0.87	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	1/6/23/26	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
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	FUC	H	3	5	-	-	0/1/1/1
6	NAG	I	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	3	BMA	O5-C5	2.93	1.49	1.43
4	F	2	NAG	O5-C5	2.82	1.48	1.43
4	E	2	NAG	O5-C5	2.74	1.48	1.43
6	I	2	NAG	O5-C5	2.66	1.48	1.43
4	D	2	NAG	O5-C5	2.56	1.48	1.43
4	F	1	NAG	O5-C5	2.43	1.48	1.43
4	G	2	NAG	O5-C5	2.41	1.48	1.43
4	G	1	NAG	O5-C5	2.39	1.48	1.43
4	D	1	NAG	O5-C5	2.36	1.48	1.43
4	D	2	NAG	C1-C2	2.35	1.55	1.52
4	E	1	NAG	O5-C5	2.29	1.47	1.43
6	I	1	NAG	O5-C5	2.26	1.47	1.43
6	I	3	BMA	O5-C1	2.21	1.47	1.43
4	G	2	NAG	O5-C1	2.18	1.47	1.43
4	E	2	NAG	O5-C1	2.17	1.47	1.43
6	I	2	NAG	O4-C4	2.07	1.48	1.43
4	F	2	NAG	O5-C1	2.06	1.47	1.43
4	G	1	NAG	O4-C4	2.04	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	3.84	117.33	112.19
4	G	2	NAG	C1-O5-C5	2.66	115.75	112.19
6	I	3	BMA	C1-O5-C5	2.63	115.71	112.19
4	E	2	NAG	C1-O5-C5	2.52	115.57	112.19
4	F	1	NAG	O4-C4-C3	-2.25	105.06	110.38
4	D	1	NAG	C1-O5-C5	2.23	115.17	112.19
4	D	1	NAG	O5-C1-C2	-2.22	107.85	111.29
6	I	1	NAG	C1-O5-C5	2.20	115.14	112.19
4	D	1	NAG	C1-C2-N2	2.20	113.89	110.43
4	F	1	NAG	O5-C1-C2	-2.12	108.02	111.29

There are no chirality outliers.

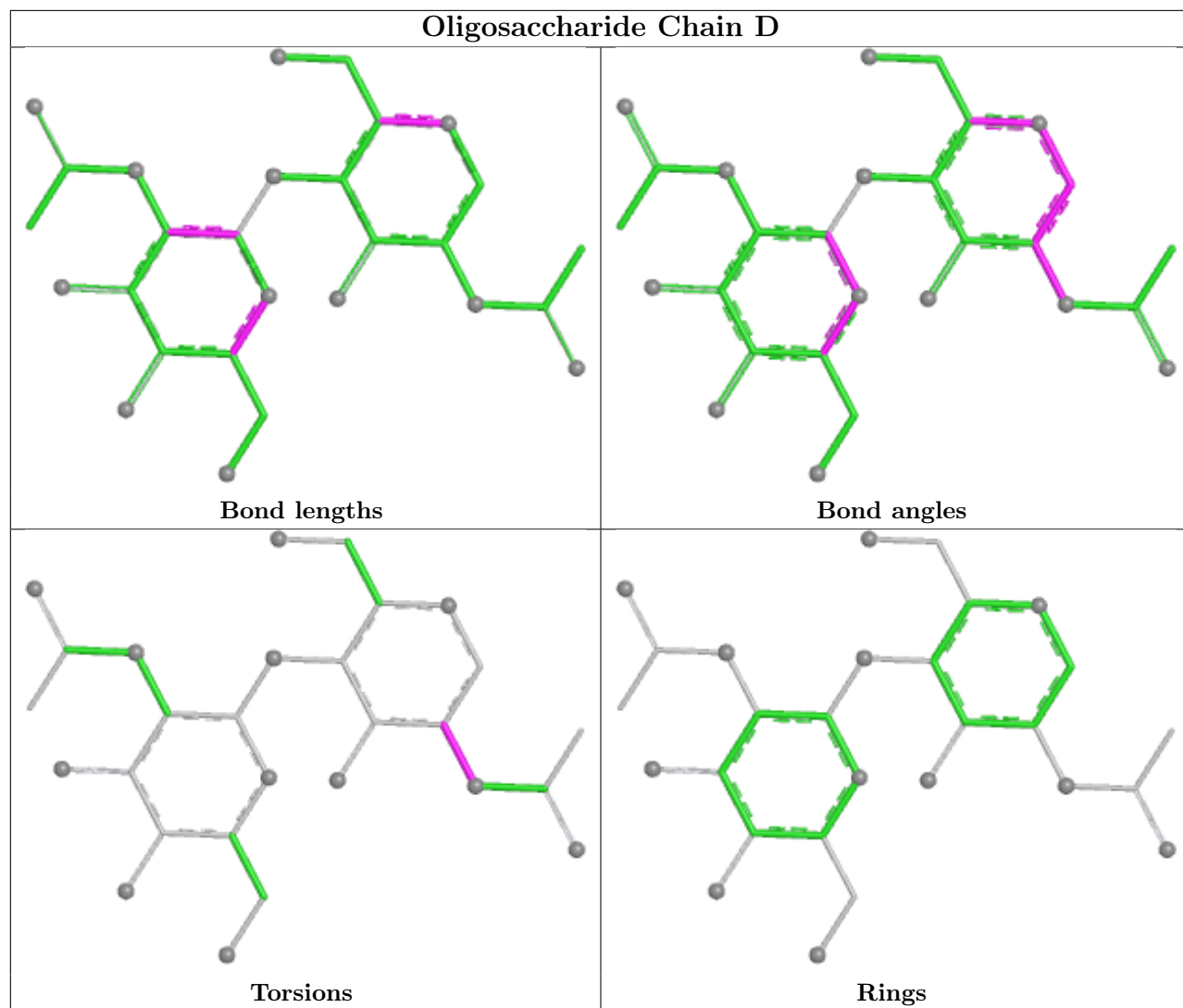
All (5) torsion outliers are listed below:

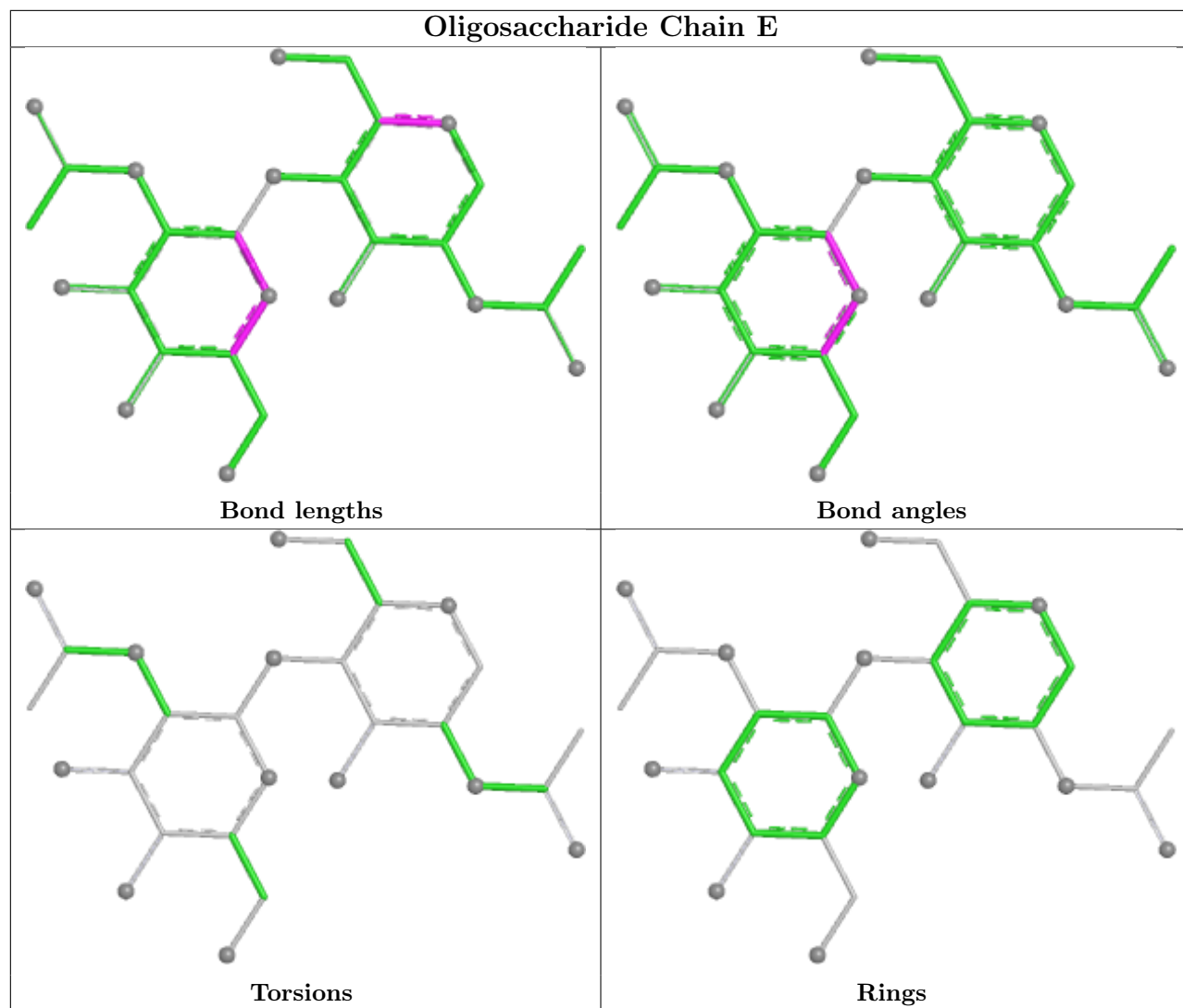
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C1-C2-N2-C7
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7

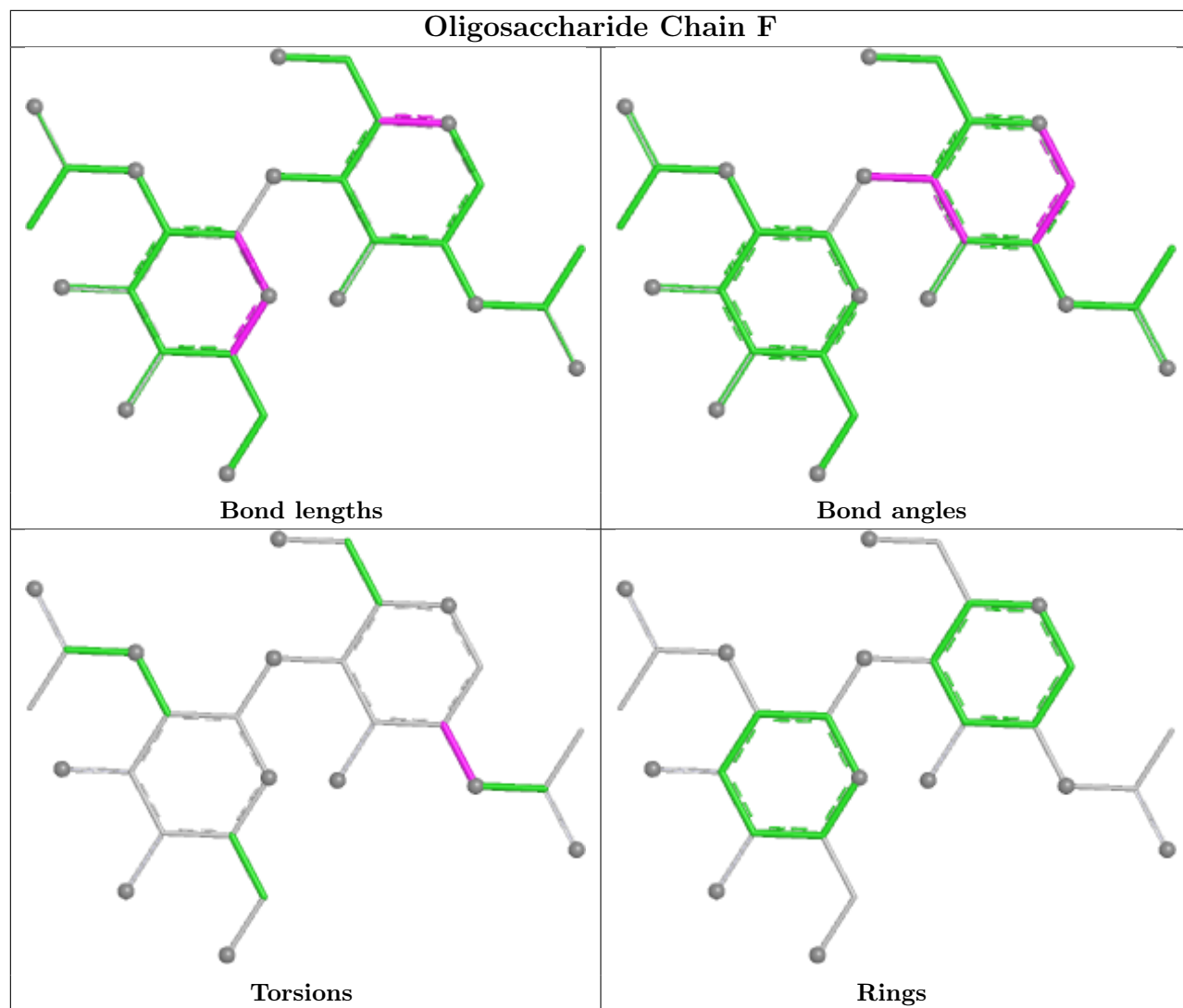
There are no ring outliers.

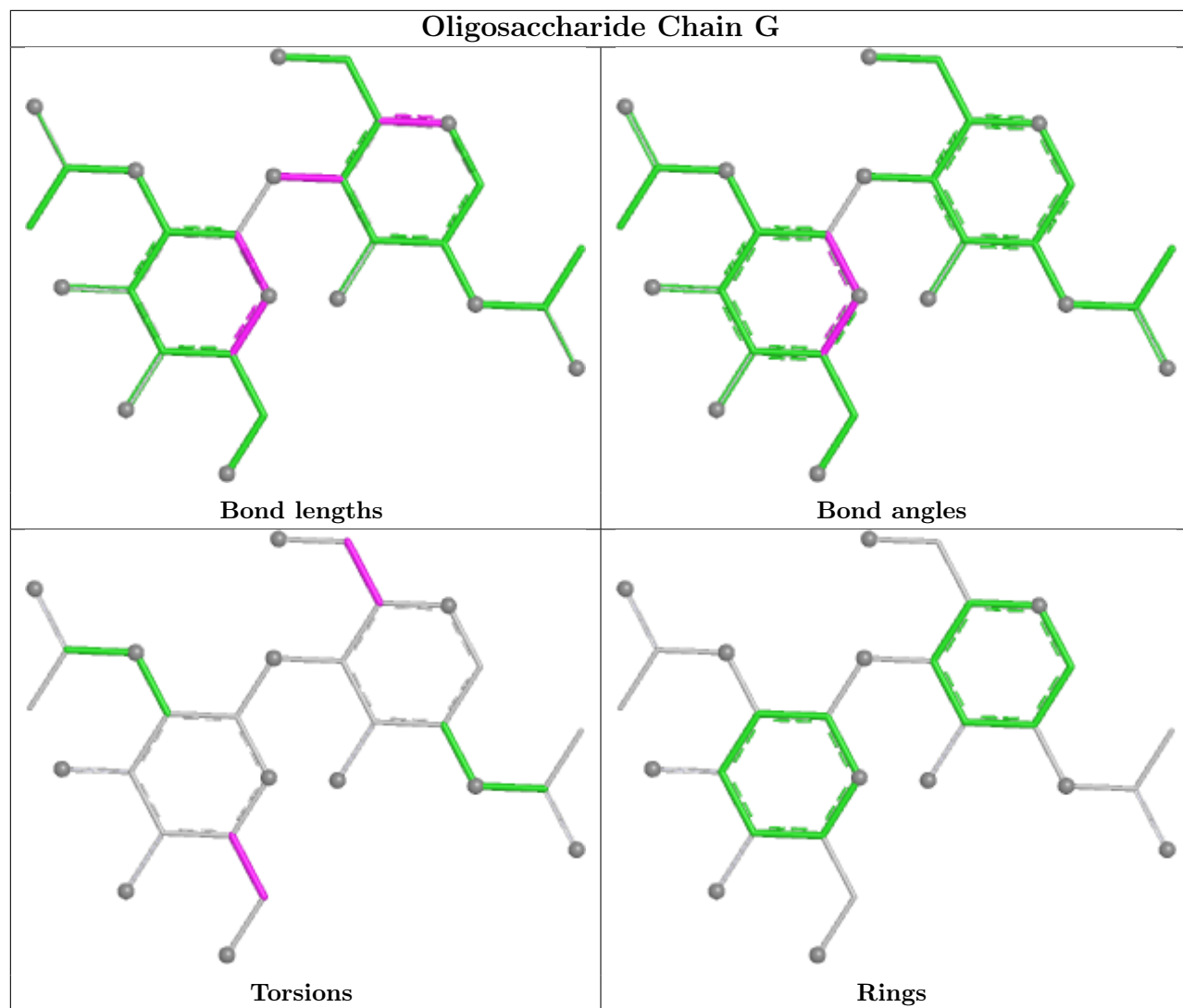
No monomer is involved in short contacts.

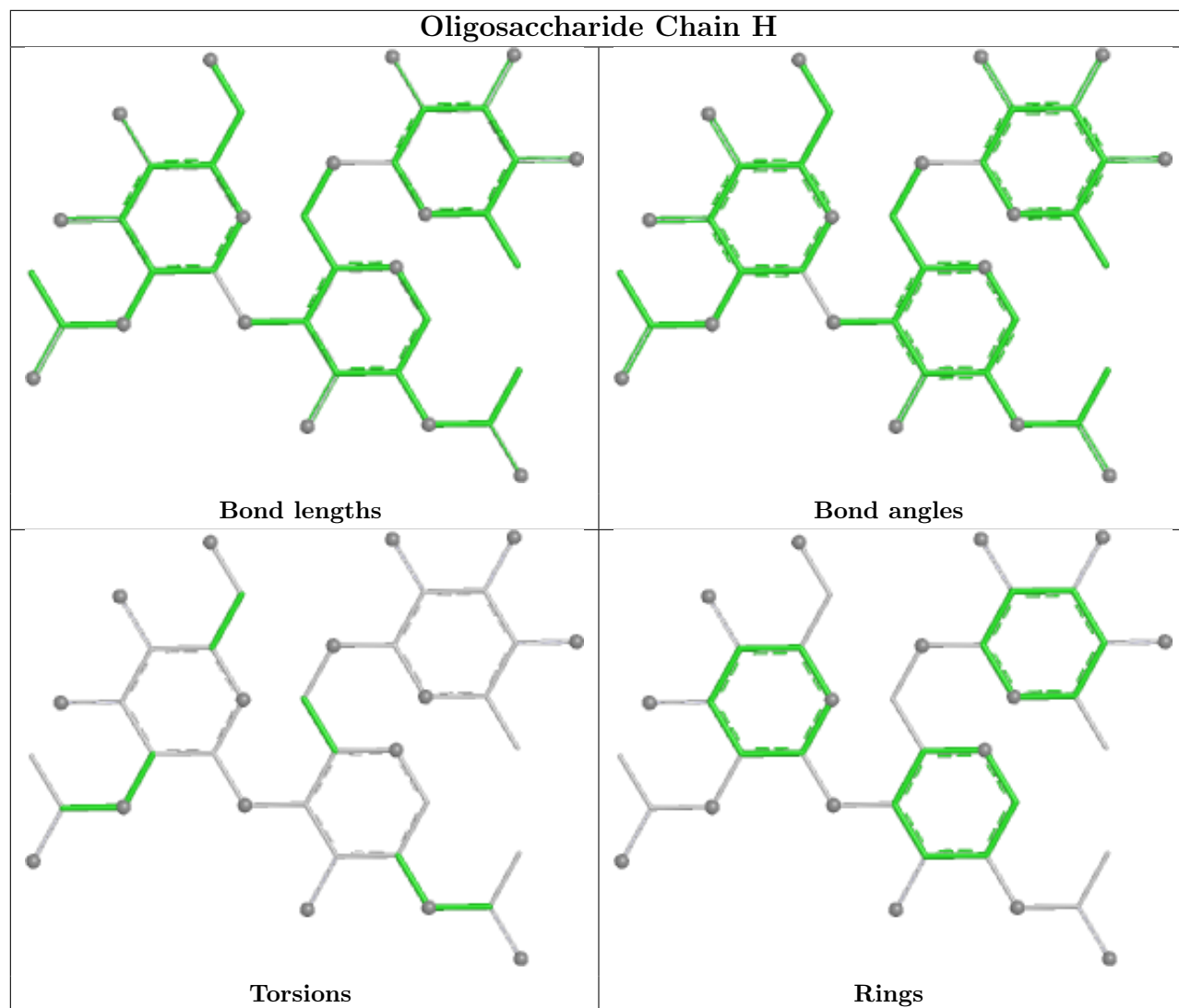
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

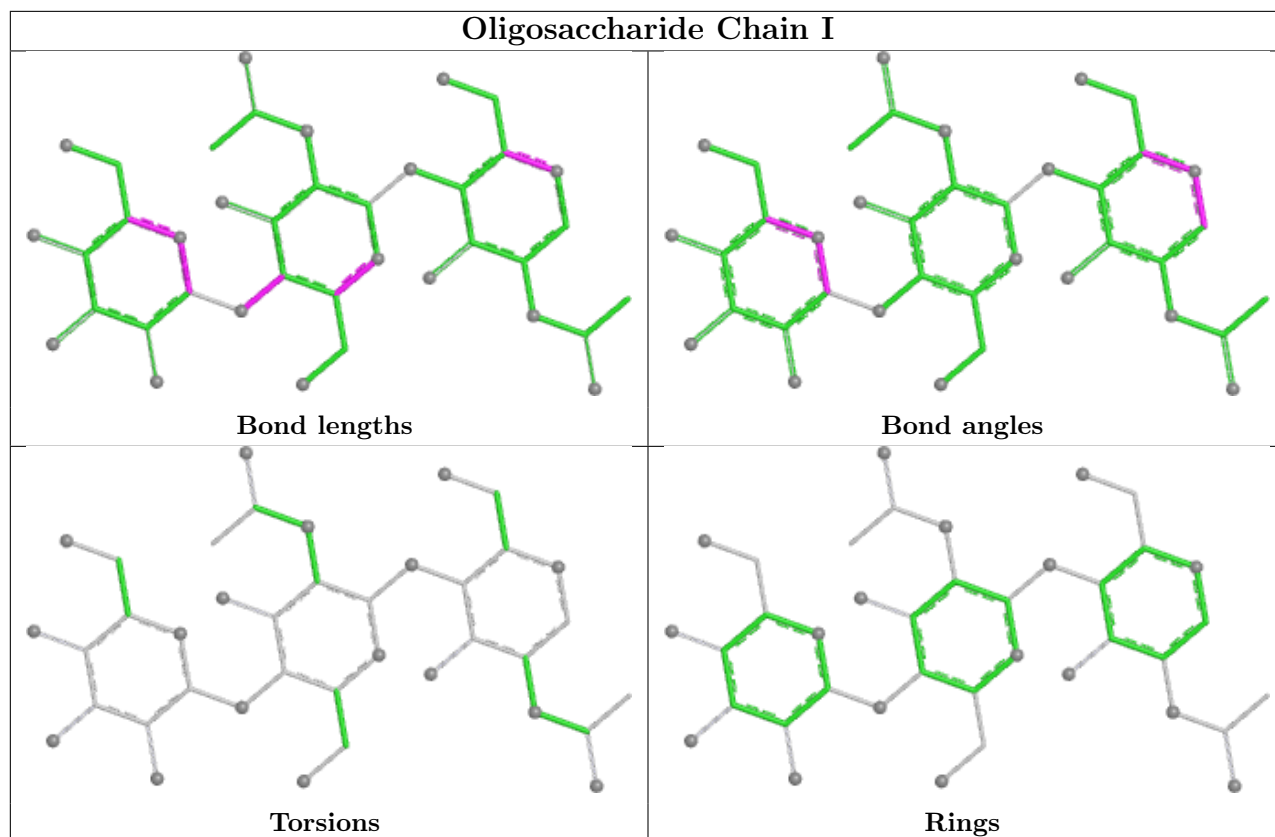












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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$
7	NAG	C	602	3	14,14,15	1.35	2 (14%)	17,19,21	1.09	1 (5%)
7	NAG	A	1004	1	14,14,15	1.35	3 (21%)	17,19,21	0.76	1 (5%)
7	NAG	A	1001	1	14,14,15	0.38	0	17,19,21	0.91	2 (11%)
7	NAG	C	601	3	14,14,15	1.24	2 (14%)	17,19,21	0.72	1 (5%)
7	NAG	C	603	3	14,14,15	1.35	3 (21%)	17,19,21	0.81	1 (5%)
7	NAG	C	604	3	14,14,15	1.32	2 (14%)	17,19,21	0.77	1 (5%)
7	NAG	A	1005	1	14,14,15	1.32	2 (14%)	17,19,21	0.83	1 (5%)
7	NAG	A	1002	1	14,14,15	1.34	3 (21%)	17,19,21	0.85	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	602	3	-	2/6/23/26	0/1/1/1
7	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	C	601	3	-	0/6/23/26	0/1/1/1
7	NAG	C	603	3	-	0/6/23/26	0/1/1/1
7	NAG	C	604	3	-	0/6/23/26	0/1/1/1
7	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1002	1	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	602	NAG	O5-C5	3.06	1.49	1.43
7	A	1005	NAG	O5-C5	2.89	1.49	1.43
7	A	1004	NAG	O5-C5	2.88	1.49	1.43
7	C	604	NAG	O5-C5	2.86	1.49	1.43
7	C	603	NAG	O5-C5	2.82	1.48	1.43
7	A	1002	NAG	O5-C5	2.81	1.48	1.43
7	C	601	NAG	O5-C5	2.67	1.48	1.43
7	A	1002	NAG	C1-C2	2.25	1.55	1.52
7	C	602	NAG	C1-C2	2.24	1.55	1.52
7	C	603	NAG	C1-C2	2.20	1.55	1.52
7	C	601	NAG	C1-C2	2.19	1.55	1.52
7	A	1004	NAG	C1-C2	2.16	1.55	1.52
7	C	604	NAG	C1-C2	2.13	1.55	1.52
7	A	1005	NAG	C1-C2	2.09	1.55	1.52
7	C	603	NAG	O5-C1	2.07	1.47	1.43
7	A	1004	NAG	O5-C1	2.02	1.47	1.43
7	A	1002	NAG	O5-C1	2.00	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1002	NAG	C1-O5-C5	2.56	115.61	112.19
7	A	1005	NAG	C1-O5-C5	2.47	115.49	112.19
7	C	603	NAG	C1-O5-C5	2.35	115.34	112.19
7	A	1004	NAG	C1-O5-C5	2.25	115.20	112.19
7	C	604	NAG	C1-O5-C5	2.11	115.02	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	601	NAG	C1-O5-C5	2.02	114.89	112.19
7	A	1001	NAG	C4-C3-C2	-2.01	108.07	111.02
7	A	1001	NAG	C2-N2-C7	2.01	125.59	122.90
7	C	602	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	602	NAG	C1-C2-N2-C7
7	A	1001	NAG	C3-C2-N2-C7
7	C	602	NAG	C3-C2-N2-C7
7	A	1001	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

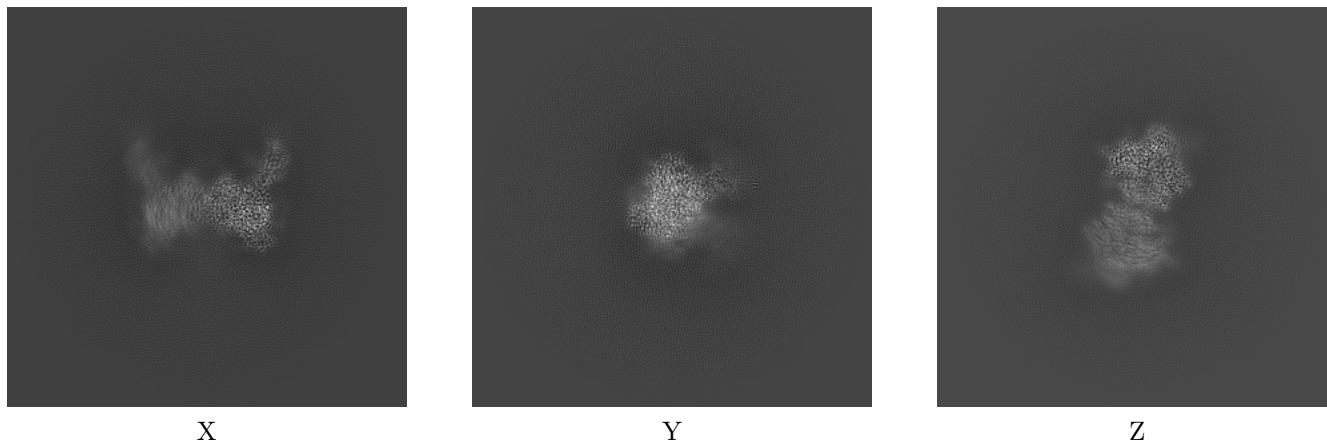
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70927. These allow visual inspection of the internal detail of the map and identification of artifacts.

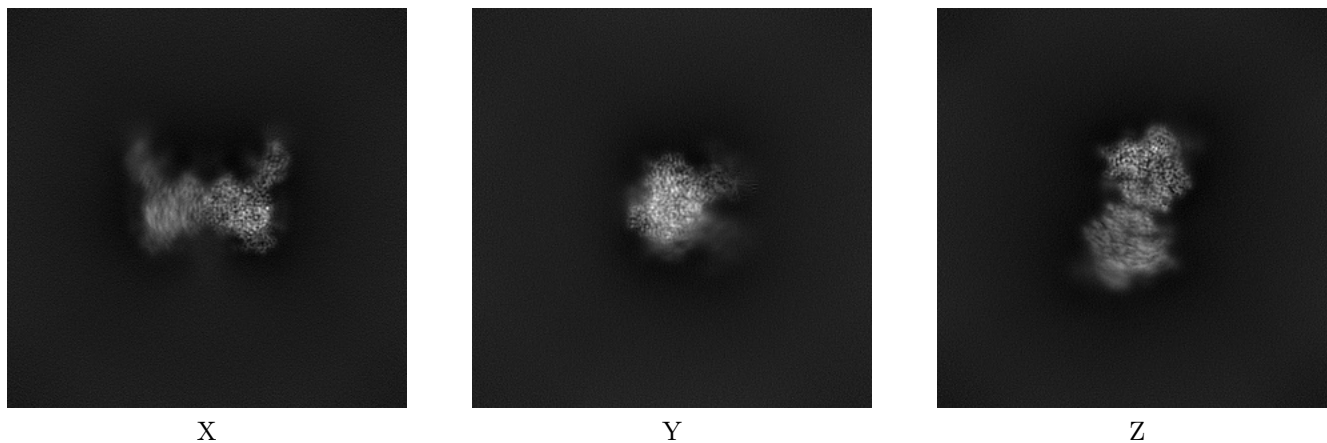
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



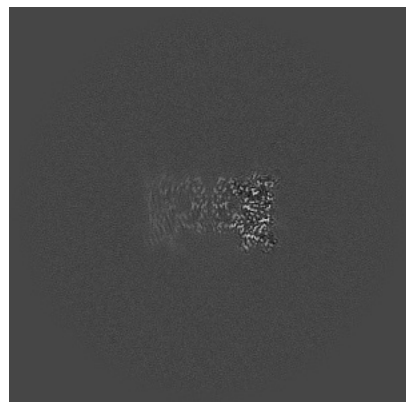
6.1.2 Raw map



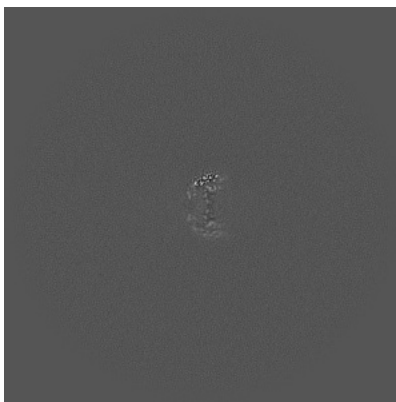
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

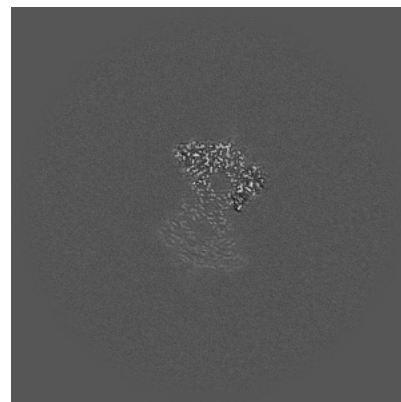
6.2.1 Primary map



X Index: 256

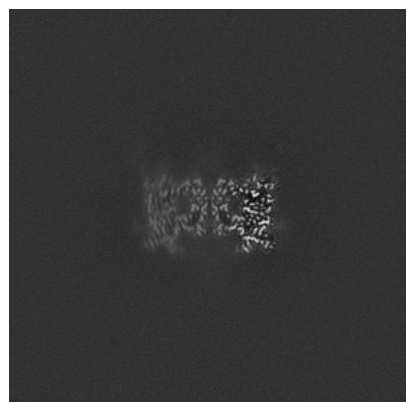


Y Index: 256

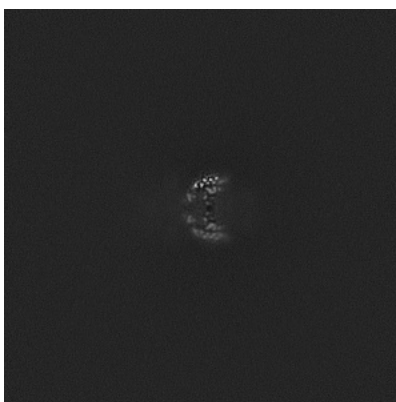


Z Index: 256

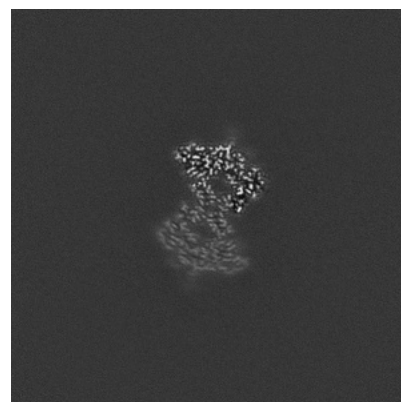
6.2.2 Raw map



X Index: 256



Y Index: 256

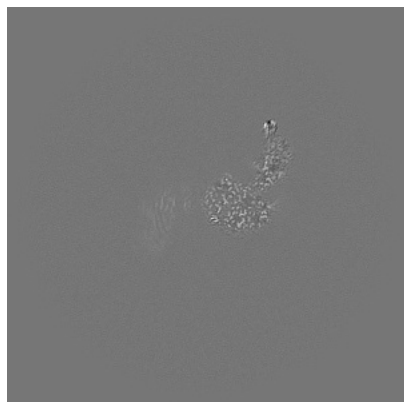


Z Index: 256

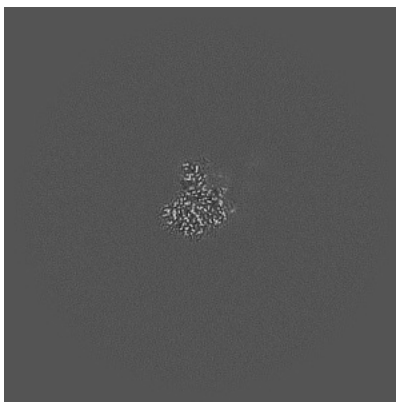
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

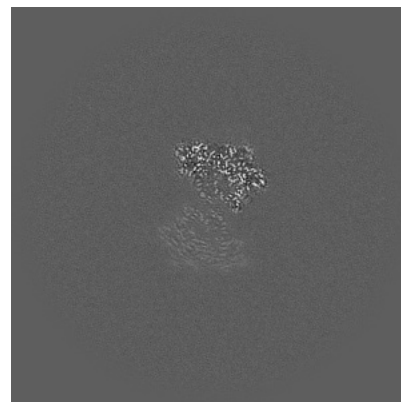
6.3.1 Primary map



X Index: 280

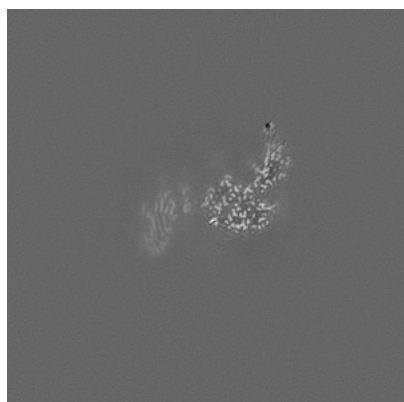


Y Index: 309

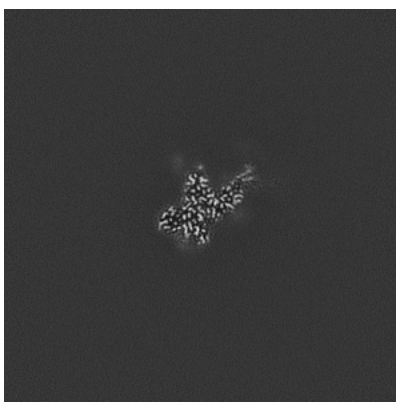


Z Index: 249

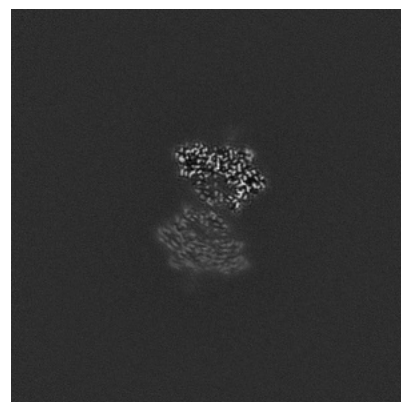
6.3.2 Raw map



X Index: 279



Y Index: 324

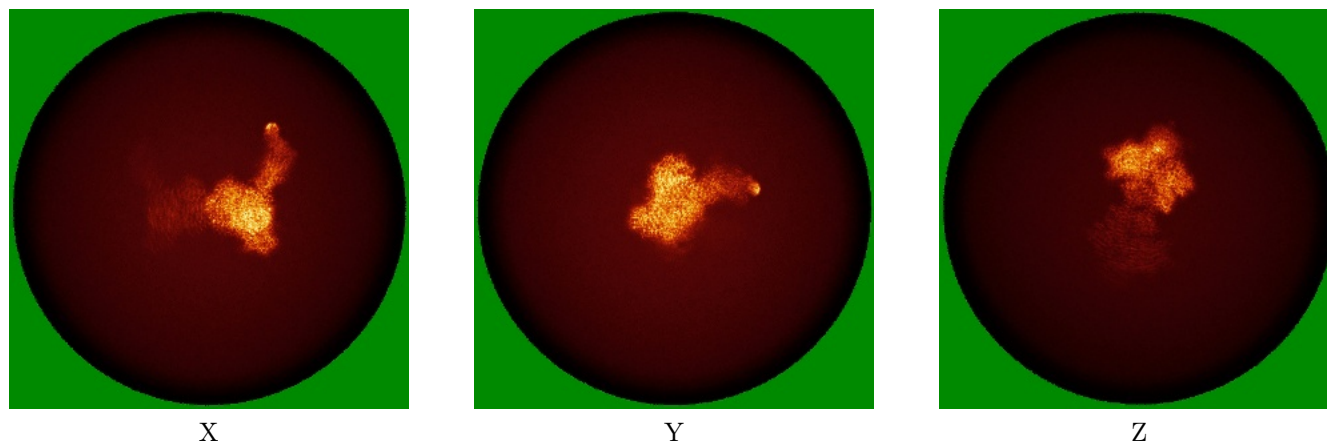


Z Index: 250

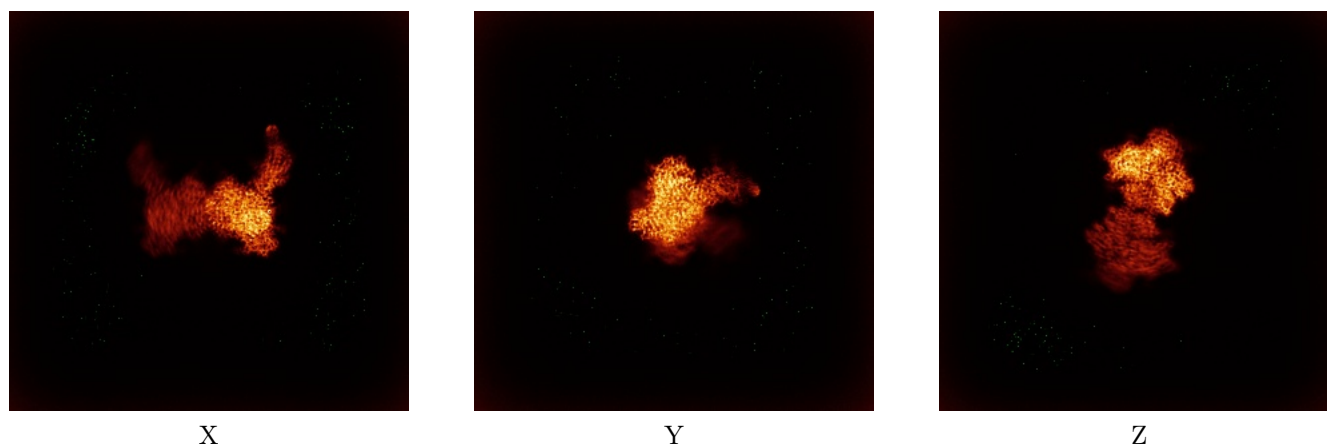
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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



X



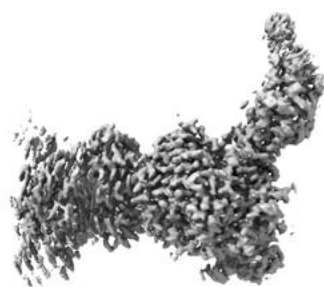
Y



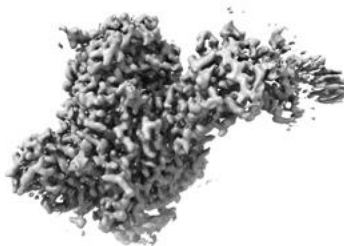
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

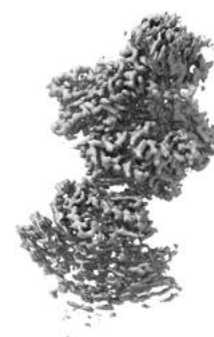
6.5.2 Raw map



X



Y



Z

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.

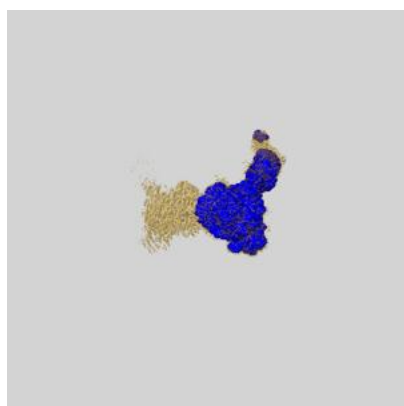
6.6 Mask visualisation [i](#)

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

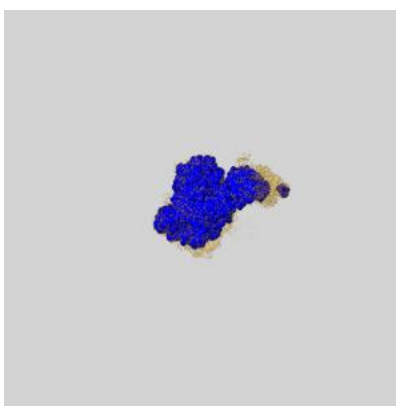
A mask typically either:

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

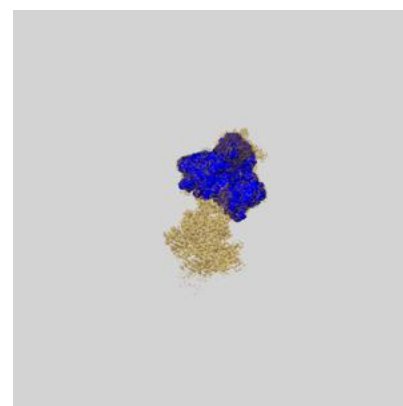
6.6.1 emd_70927_msk_1.map [i](#)



X



Y

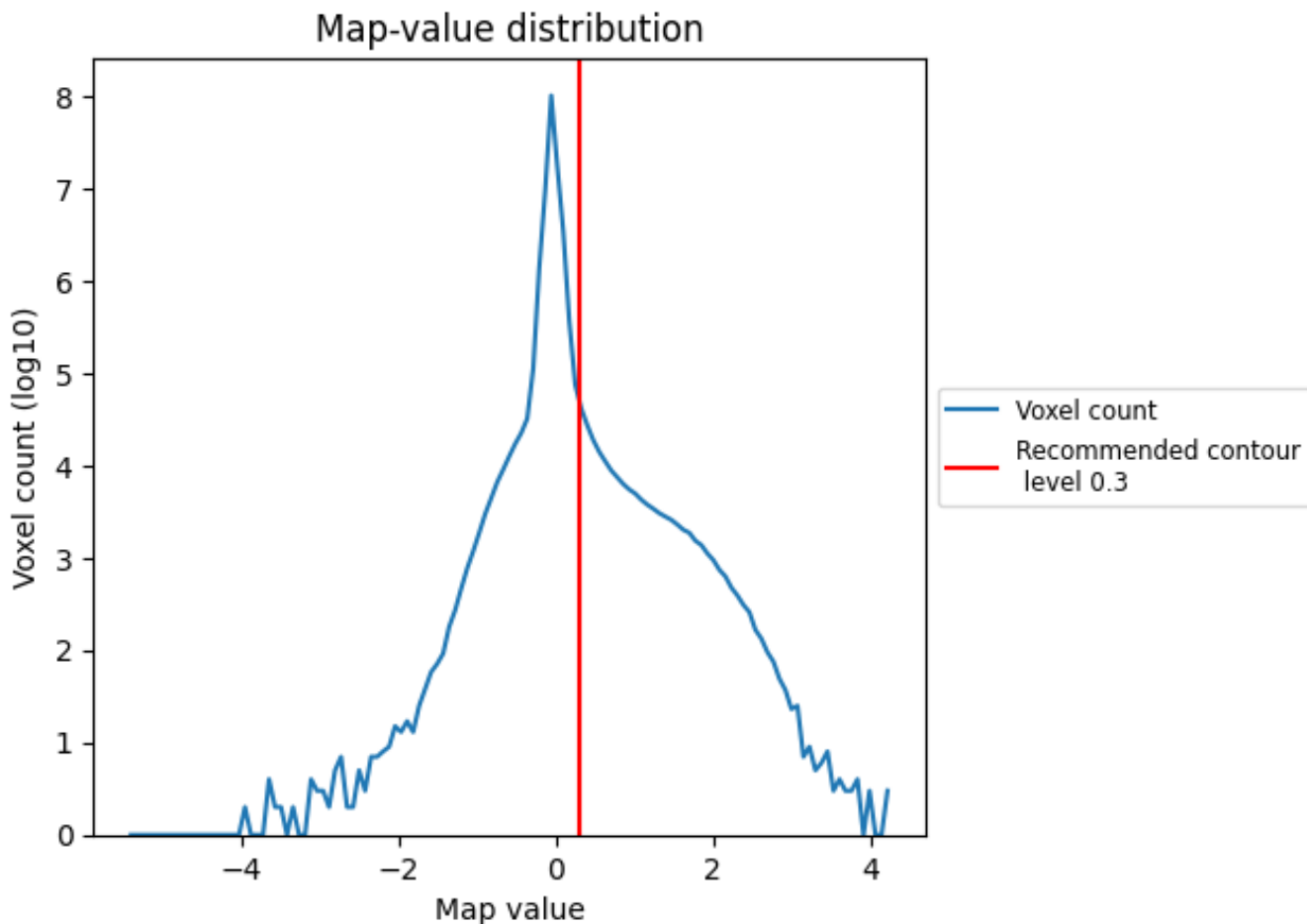


Z

7 Map analysis [i](#)

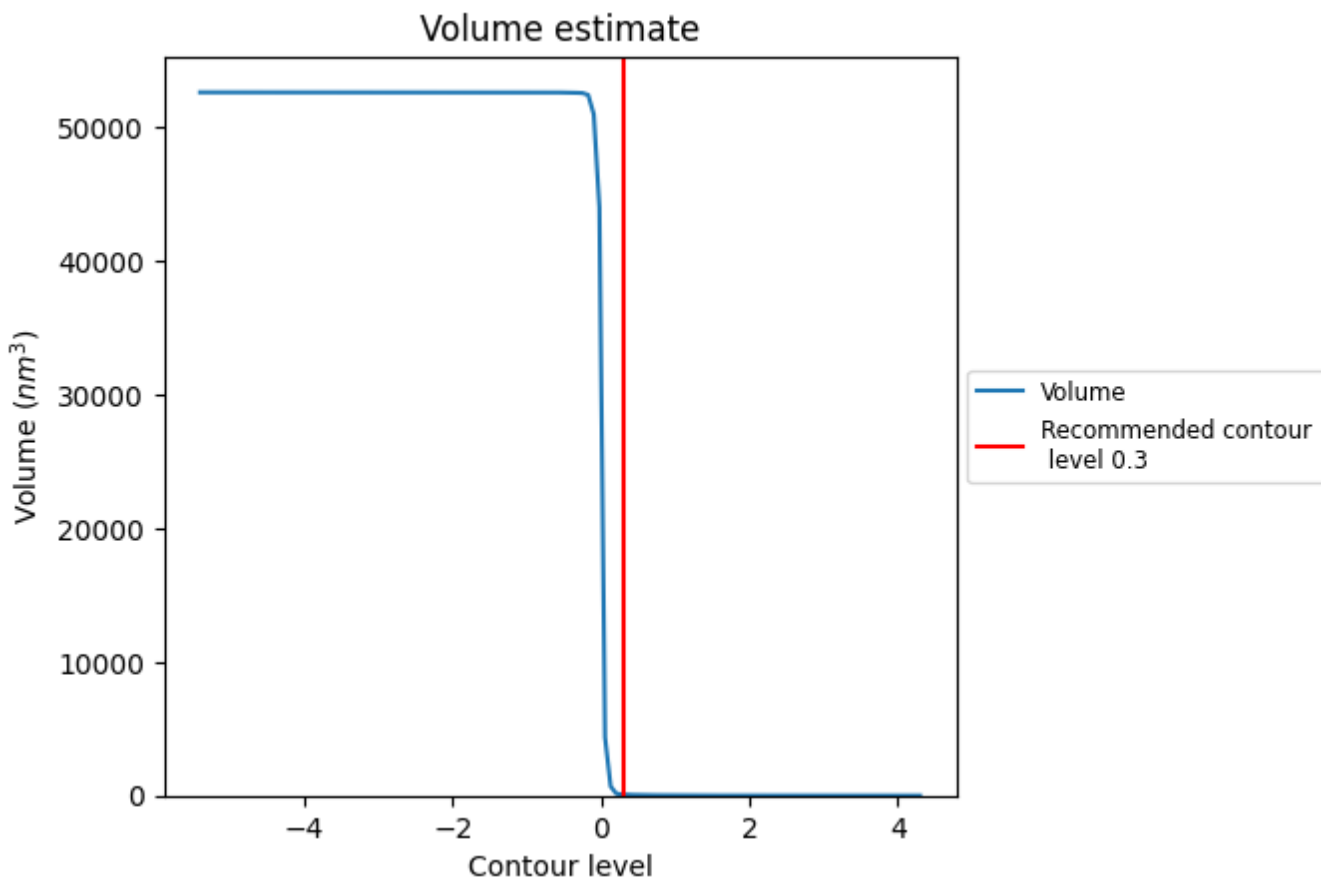
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

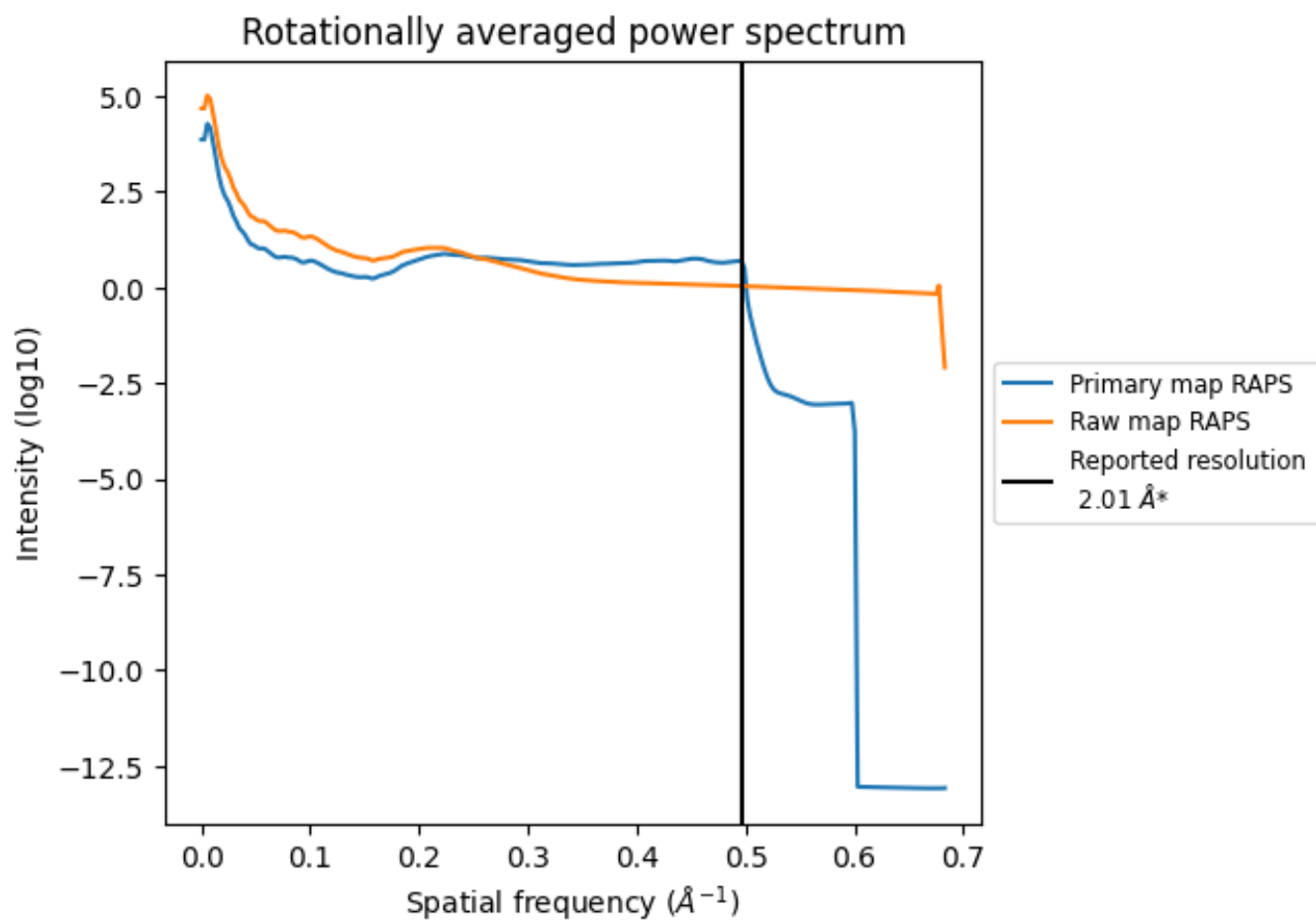
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 72 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

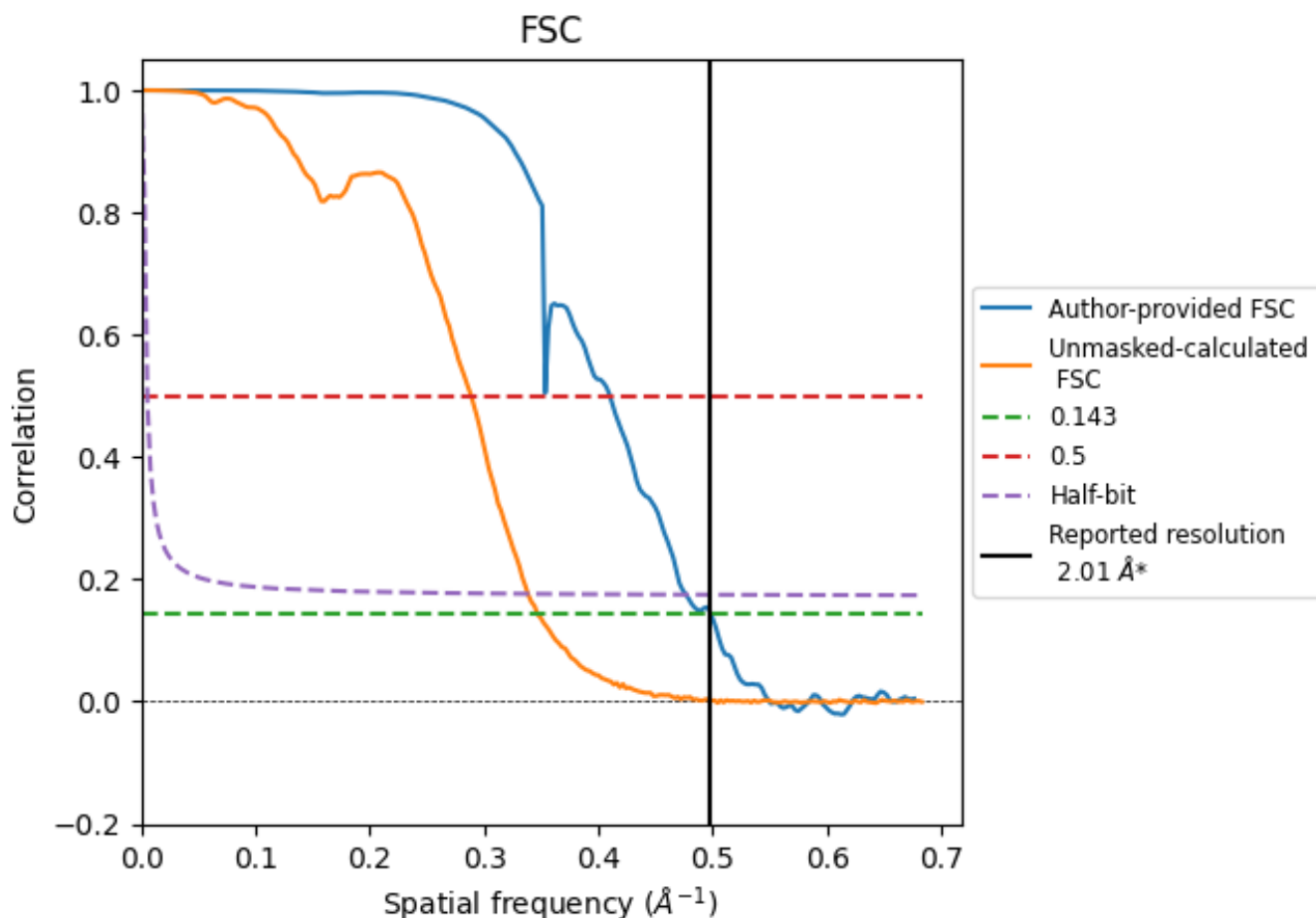


*Reported resolution corresponds to spatial frequency of 0.498 Å⁻¹

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 0.498\AA^{-1}

8.2 Resolution estimates [i](#)

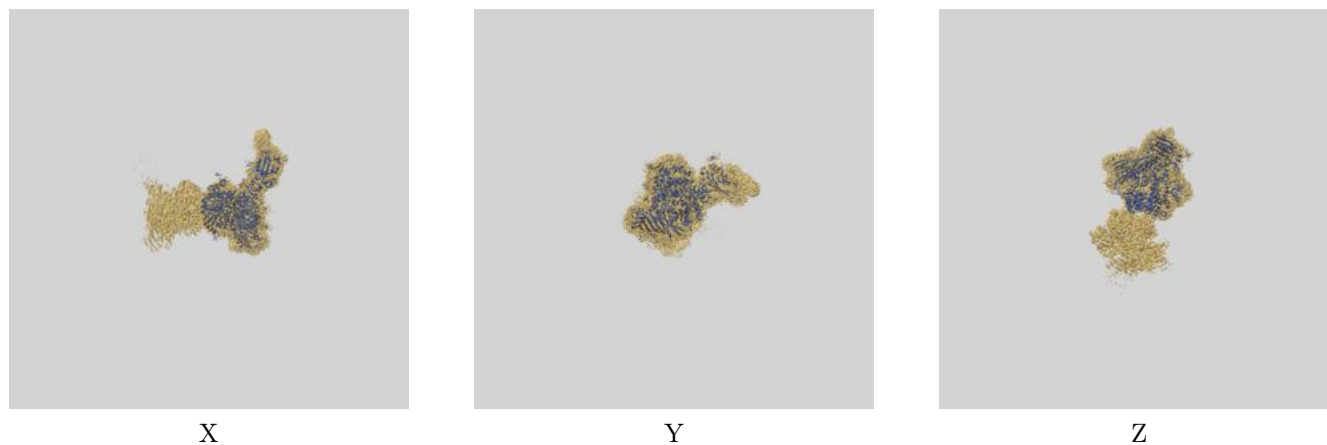
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.44	2.10
Unmasked-calculated*	2.88	3.47	2.96

*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 2.88 differs from the reported value 2.01 by more than 10 %

9 Map-model fit [i](#)

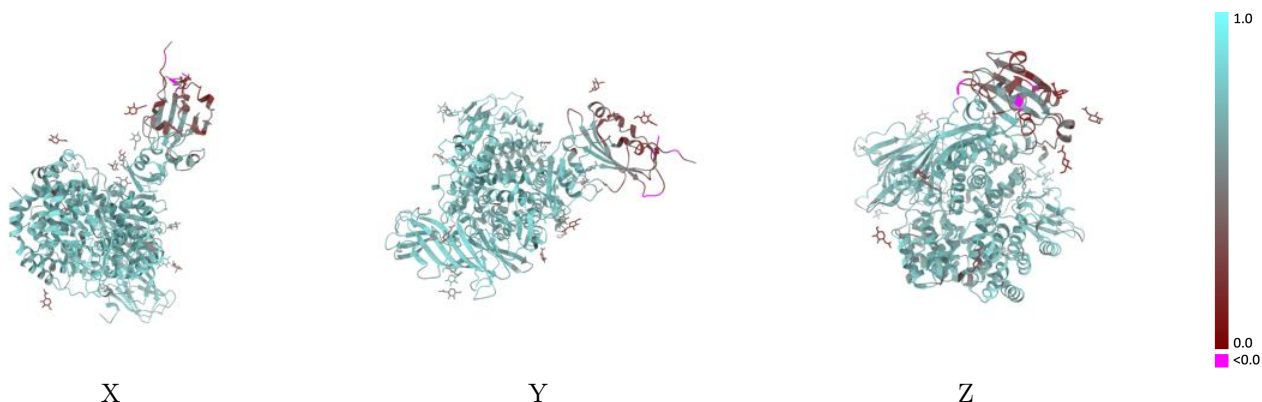
This section contains information regarding the fit between EMDB map EMD-70927 and PDB model 9OW3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



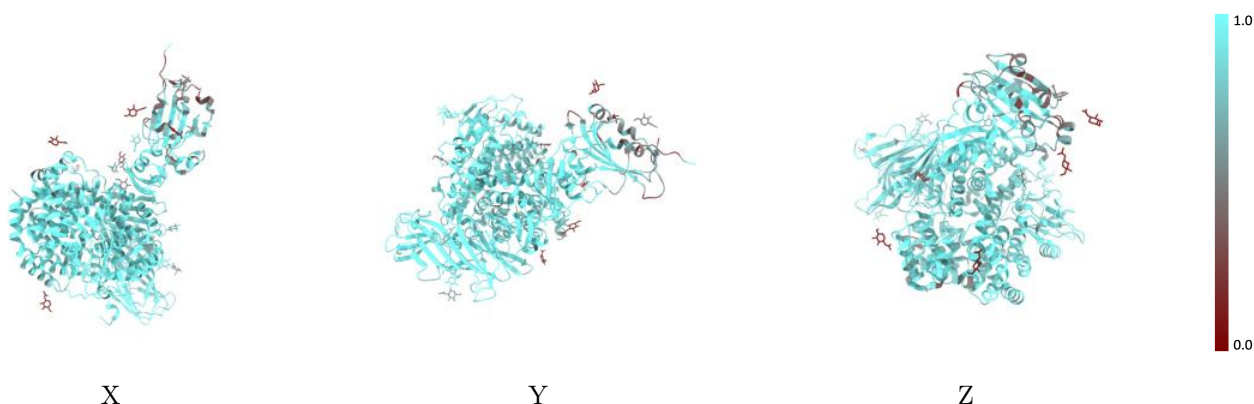
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



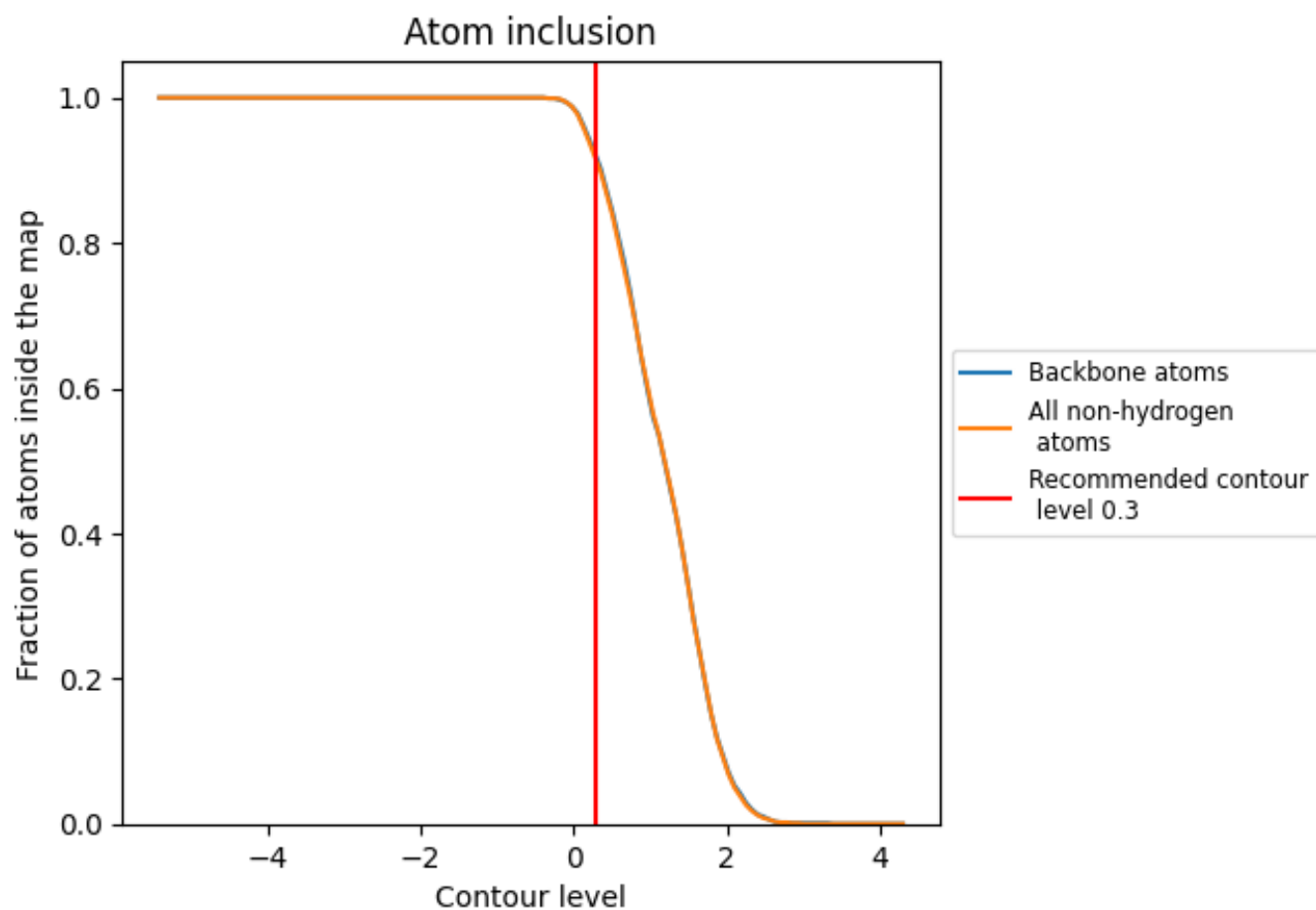
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.6830
A	 0.9480	 0.7240
B	 0.6970	 0.4980
C	 0.7850	 0.5240
D	 0.7500	 0.5560
E	 0.8930	 0.6100
F	 0.7860	 0.5020
G	 0.4640	 0.3160
H	 0.9210	 0.5940
I	 0.7440	 0.5890

