



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:08 AM UTC

PDB ID : 5JNX / pdb_00005jnx
EMDB ID : EMD-8169
Title : The 6.6 Å cryo-EM structure of the full-length human NPC1 in complex with the cleaved glycoprotein of Ebola virus
Authors : Gong, X.; Qian, H.W.; Zhou, X.H.; Wu, J.P.; Wan, T.; Shi, Y.; Gao, F.; Zhou, Q.; Yan, N.
Deposited on : 2016-05-01
Resolution : 6.56 Å(reported)

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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:

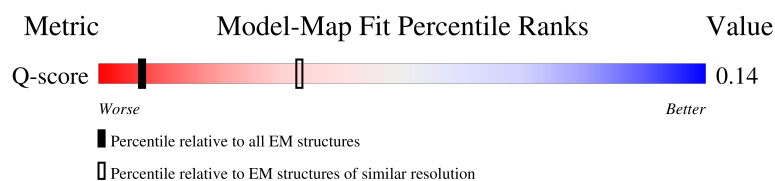
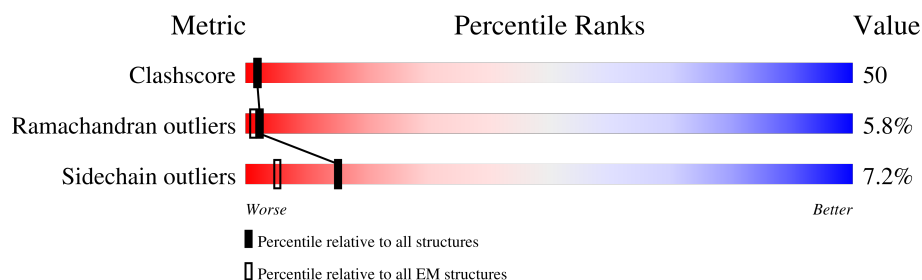
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 6.56 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	501 (6.07 - 7.06)

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	1278	
2	C	158	
2	E	158	
2	G	158	

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Mol	Chain	Length	Quality of chain
3	D	130	
3	F	130	
3	H	130	
4	B	2	
4	I	2	
4	K	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
5	J	3	
6	L	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	J	1	-	-	X	-
5	NAG	J	2	-	-	X	-
6	NAG	L	1	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13749 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 Niemann-Pick C1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1133	Total	C	N	O	S	1	0
			7695	4862	1315	1476	42		

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	158	Total	C	N	O	S	0	0
			1194	757	209	223	5		
2	E	158	Total	C	N	O	S	0	0
			1194	757	209	223	5		
2	G	158	Total	C	N	O	S	0	0
			1194	757	209	223	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	31	ARG	-	expression tag	UNP P87666
C	42	VAL	THR	engineered mutation	UNP P87666
E	31	ARG	-	expression tag	UNP P87666
E	42	VAL	THR	engineered mutation	UNP P87666
G	31	ARG	-	expression tag	UNP P87666
G	42	VAL	THR	engineered mutation	UNP P87666

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	87	Total	C	N	O	S	0	0
			687	441	121	122	3		
3	F	87	Total	C	N	O	S	0	0
			687	441	121	122	3		
3	H	87	Total	C	N	O	S	0	0
			687	441	121	122	3		

There are 18 discrepancies between the modelled and reference sequences:

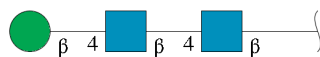
Chain	Residue	Modelled	Actual	Comment	Reference
D	633	HIS	-	expression tag	UNP P87666
D	634	HIS	-	expression tag	UNP P87666
D	635	HIS	-	expression tag	UNP P87666
D	636	HIS	-	expression tag	UNP P87666
D	637	HIS	-	expression tag	UNP P87666
D	638	HIS	-	expression tag	UNP P87666
F	633	HIS	-	expression tag	UNP P87666
F	634	HIS	-	expression tag	UNP P87666
F	635	HIS	-	expression tag	UNP P87666
F	636	HIS	-	expression tag	UNP P87666
F	637	HIS	-	expression tag	UNP P87666
F	638	HIS	-	expression tag	UNP P87666
H	633	HIS	-	expression tag	UNP P87666
H	634	HIS	-	expression tag	UNP P87666
H	635	HIS	-	expression tag	UNP P87666
H	636	HIS	-	expression tag	UNP P87666
H	637	HIS	-	expression tag	UNP P87666
H	638	HIS	-	expression tag	UNP P87666

- 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	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	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.



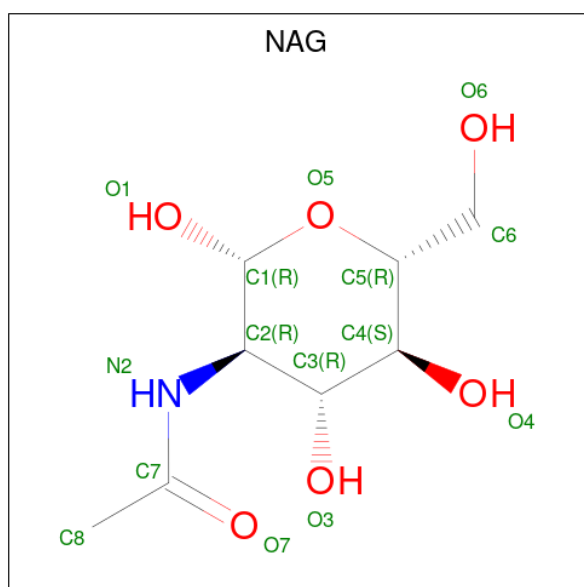
Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

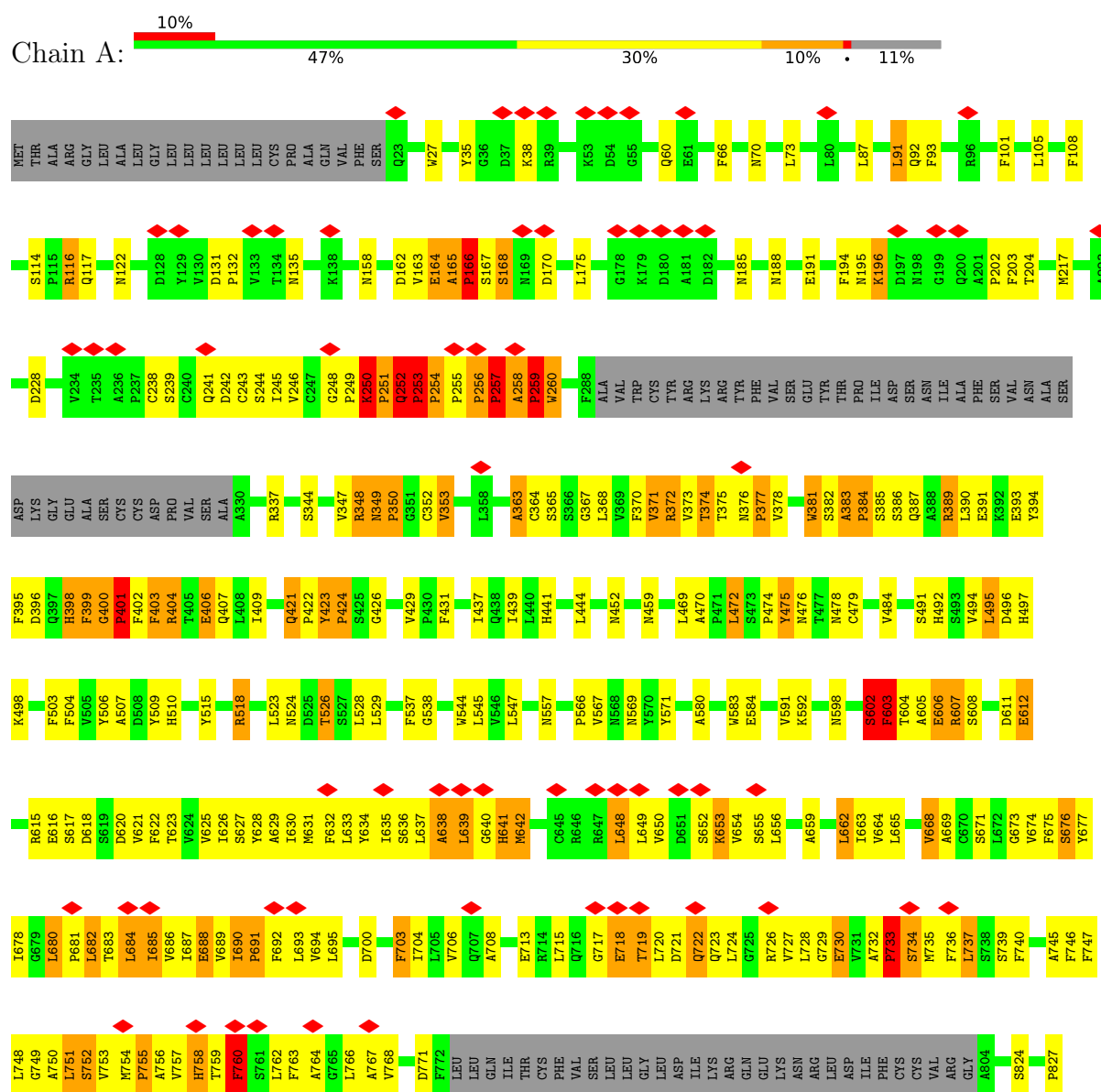


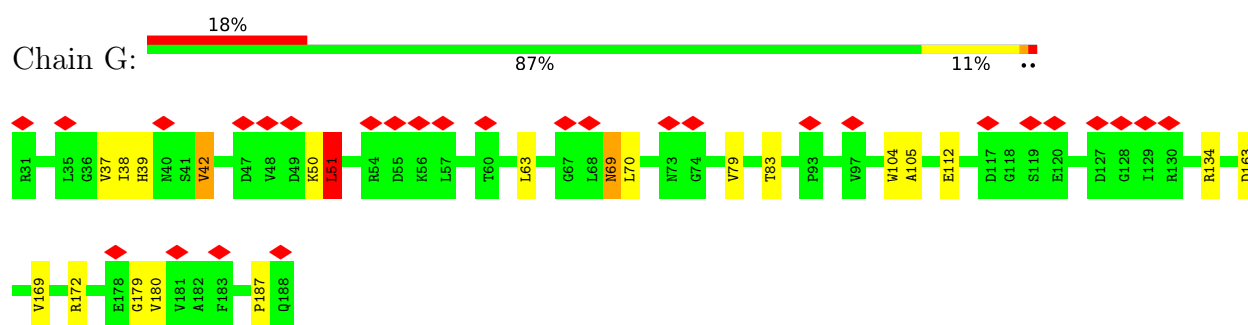
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

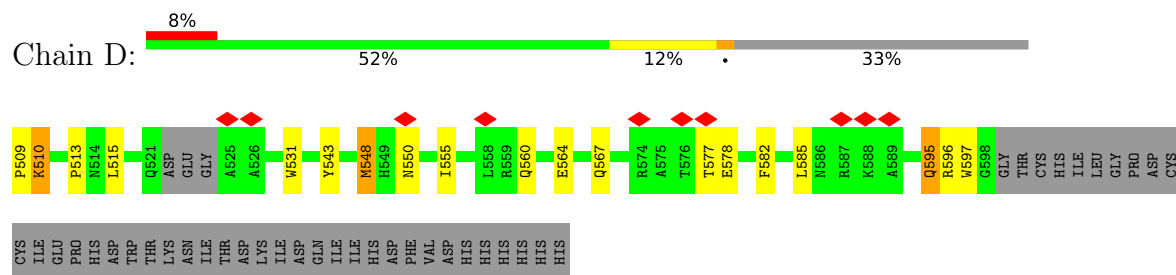
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Niemann-Pick C1 protein

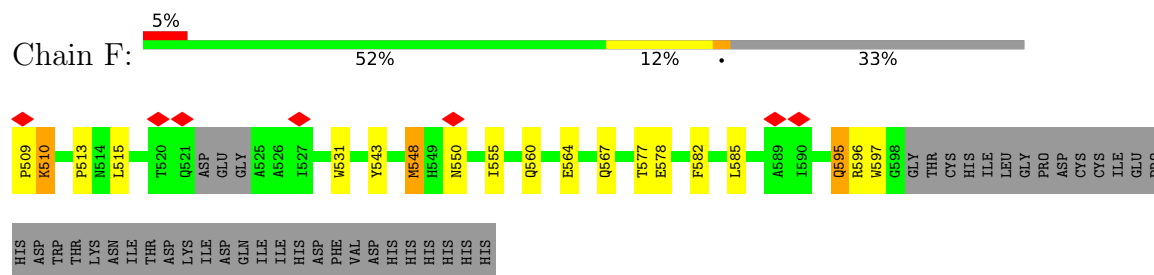




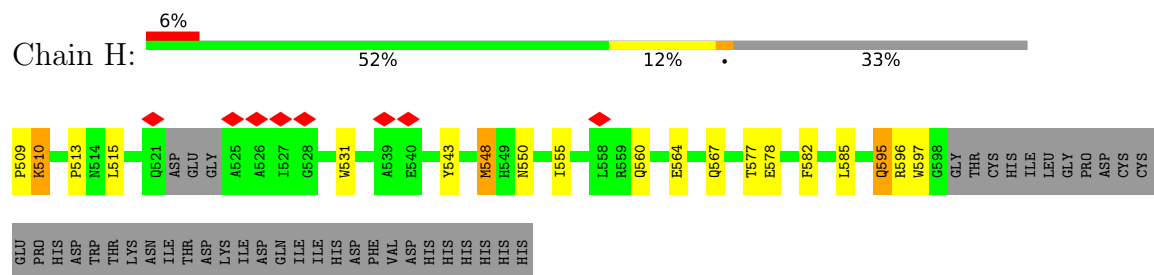
- Molecule 3: Envelope glycoprotein



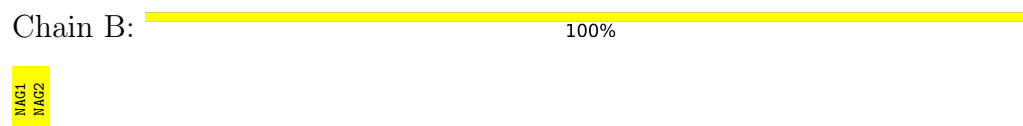
- Molecule 3: Envelope glycoprotein



- Molecule 3: Envelope 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



- 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 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

Chain J:  100%

MAG1
MAG2
BMA3

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

Chain L:  100%

MAG1
MAG2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	38270	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	334.47424, 334.47424, 334.47424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	20/7843 (0.3%)	0.97	55/10748 (0.5%)
2	C	0.55	1/1223 (0.1%)	0.86	0/1664
2	E	0.58	2/1223 (0.2%)	0.85	0/1664
2	G	0.55	1/1223 (0.1%)	0.85	0/1664
3	D	0.54	0/702	1.01	1/952 (0.1%)
3	F	0.54	0/702	1.01	1/952 (0.1%)
3	H	0.54	0/702	1.01	2/952 (0.2%)
All	All	0.60	24/13618 (0.2%)	0.95	59/18596 (0.3%)

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	2
2	C	0	1
2	E	0	1
2	G	0	1
All	All	0	5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	LEU	C-N	-9.33	1.22	1.33
1	A	1060	LEU	C-N	8.59	1.44	1.33
1	A	881	GLN	C-N	-8.29	1.22	1.33
1	A	884	HIS	C-N	-7.96	1.23	1.33
1	A	429	VAL	C-N	-7.63	1.23	1.33

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	GLN	N-CA-C	10.41	123.54	108.86
1	A	995	PHE	N-CA-C	10.38	121.93	108.34
1	A	429	VAL	O-C-N	-8.86	111.00	121.10
1	A	602	SER	CB-CA-C	-8.61	91.12	110.07
1	A	996	MET	CA-C-N	-8.60	105.12	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	602	SER	Peptide
1	A	603	PHE	Peptide
2	C	69	ASN	Sidechain
2	E	69	ASN	Sidechain
2	G	69	ASN	Sidechain

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	7695	0	6477	1163	0
2	C	1194	0	1153	18	0
2	E	1194	0	1153	71	0
2	G	1194	0	1153	17	0
3	D	687	0	679	20	0
3	F	687	0	679	21	0
3	H	687	0	679	18	0
4	B	28	0	25	0	0
4	I	28	0	25	2	0
4	K	28	0	25	4	0
4	M	28	0	25	3	0
4	N	28	0	25	1	0
4	O	28	0	25	2	0
4	P	28	0	25	1	0
5	J	39	0	34	17	0
6	L	50	0	43	9	0
7	A	126	0	117	8	0
All	All	13749	0	12342	1286	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 50.

The worst 5 of 1286 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:724:LEU:HD22	1:A:1170:HIS:CE1	1.29	1.62
1:A:656:LEU:CD1	1:A:685:ILE:HG13	1.17	1.60
1:A:1138:MET:HE2	1:A:1232:MET:CB	1.20	1.59
1:A:656:LEU:HD11	1:A:685:ILE:CG1	1.31	1.58
1:A:598:ASN:HD21	4:K:1:NAG:C1	0.99	1.57

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	1126/1278 (88%)	897 (80%)	135 (12%)	94 (8%)	0	9
2	C	156/158 (99%)	142 (91%)	12 (8%)	2 (1%)	9	42
2	E	156/158 (99%)	141 (90%)	13 (8%)	2 (1%)	9	42
2	G	156/158 (99%)	142 (91%)	12 (8%)	2 (1%)	9	42
3	D	83/130 (64%)	77 (93%)	4 (5%)	2 (2%)	4	27
3	F	83/130 (64%)	77 (93%)	4 (5%)	2 (2%)	4	27
3	H	83/130 (64%)	77 (93%)	4 (5%)	2 (2%)	4	27
All	All	1843/2142 (86%)	1553 (84%)	184 (10%)	106 (6%)	2	13

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	LYS
1	A	256	PRO

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Mol	Chain	Res	Type
1	A	350	PRO
1	A	372	ARG
1	A	374	THR

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	643/1109 (58%)	567 (88%)	76 (12%)	5	18
2	C	126/130 (97%)	124 (98%)	2 (2%)	55	70
2	E	126/130 (97%)	124 (98%)	2 (2%)	55	70
2	G	126/130 (97%)	124 (98%)	2 (2%)	55	70
3	D	70/111 (63%)	68 (97%)	2 (3%)	37	58
3	F	70/111 (63%)	68 (97%)	2 (3%)	37	58
3	H	70/111 (63%)	68 (97%)	2 (3%)	37	58
All	All	1231/1832 (67%)	1143 (93%)	88 (7%)	15	35

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1090	GLN
1	A	1199	PHE
1	A	1127	MET
1	A	1166	GLU
1	A	1234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	598	ASN
3	H	595	GLN
2	C	39	HIS
2	G	39	HIS

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Mol	Chain	Res	Type
1	A	1072	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 ⓘ

21 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	4,1	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
4	NAG	B	2	4	14,14,15	0.55	0	17,19,21	0.74	1 (5%)
4	NAG	I	1	4,1	14,14,15	0.48	0	17,19,21	1.47	3 (17%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.57	0
5	NAG	J	1	5,1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	J	2	5	14,14,15	0.29	0	17,19,21	0.56	0
5	BMA	J	3	5	11,11,12	0.26	0	15,15,17	0.52	0
4	NAG	K	1	4,1	14,14,15	0.36	0	17,19,21	1.56	3 (17%)
4	NAG	K	2	4	14,14,15	0.68	1 (7%)	17,19,21	1.06	1 (5%)
6	NAG	L	1	1,6	14,14,15	0.28	0	17,19,21	0.56	0
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.78	0
6	BMA	L	3	6	11,11,12	0.28	0	15,15,17	0.64	0
6	MAN	L	4	6	11,11,12	0.35	0	15,15,17	1.02	1 (6%)
4	NAG	M	1	4,1	14,14,15	0.41	0	17,19,21	1.15	2 (11%)
4	NAG	M	2	4	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
4	NAG	N	1	3,4	14,14,15	0.71	1 (7%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	O	1	3,4	14,14,15	0.72	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	O	2	4	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	P	1	3,4	14,14,15	0.71	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	P	2	4	14,14,15	0.30	0	17,19,21	0.57	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
4	NAG	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
6	MAN	L	4	6	-	2/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	NAG	O	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
4	NAG	P	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	1	NAG	C2-N2	2.09	1.49	1.46
4	P	1	NAG	C2-N2	2.08	1.49	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	NAG	C1-C2	2.07	1.55	1.52
4	N	1	NAG	C2-N2	2.05	1.49	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	O5-C1-C2	-4.37	104.53	111.29
4	K	1	NAG	C1-O5-C5	3.47	116.83	112.19
4	K	1	NAG	O4-C4-C3	-3.24	102.75	110.38
4	N	1	NAG	O5-C1-C2	-3.10	106.50	111.29
4	P	1	NAG	O5-C1-C2	-3.09	106.50	111.29

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C1-C2-N2-C7
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2

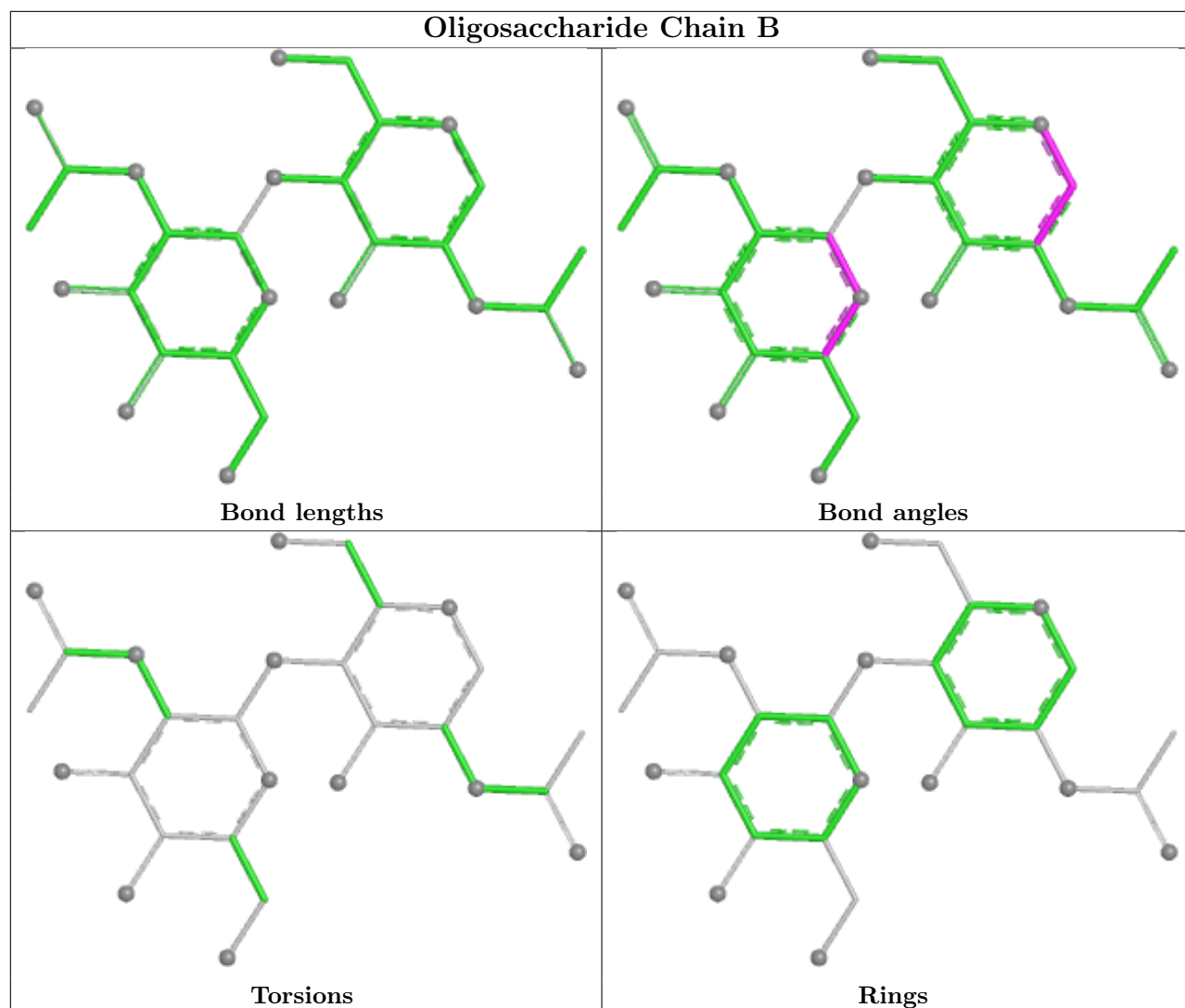
There are no ring outliers.

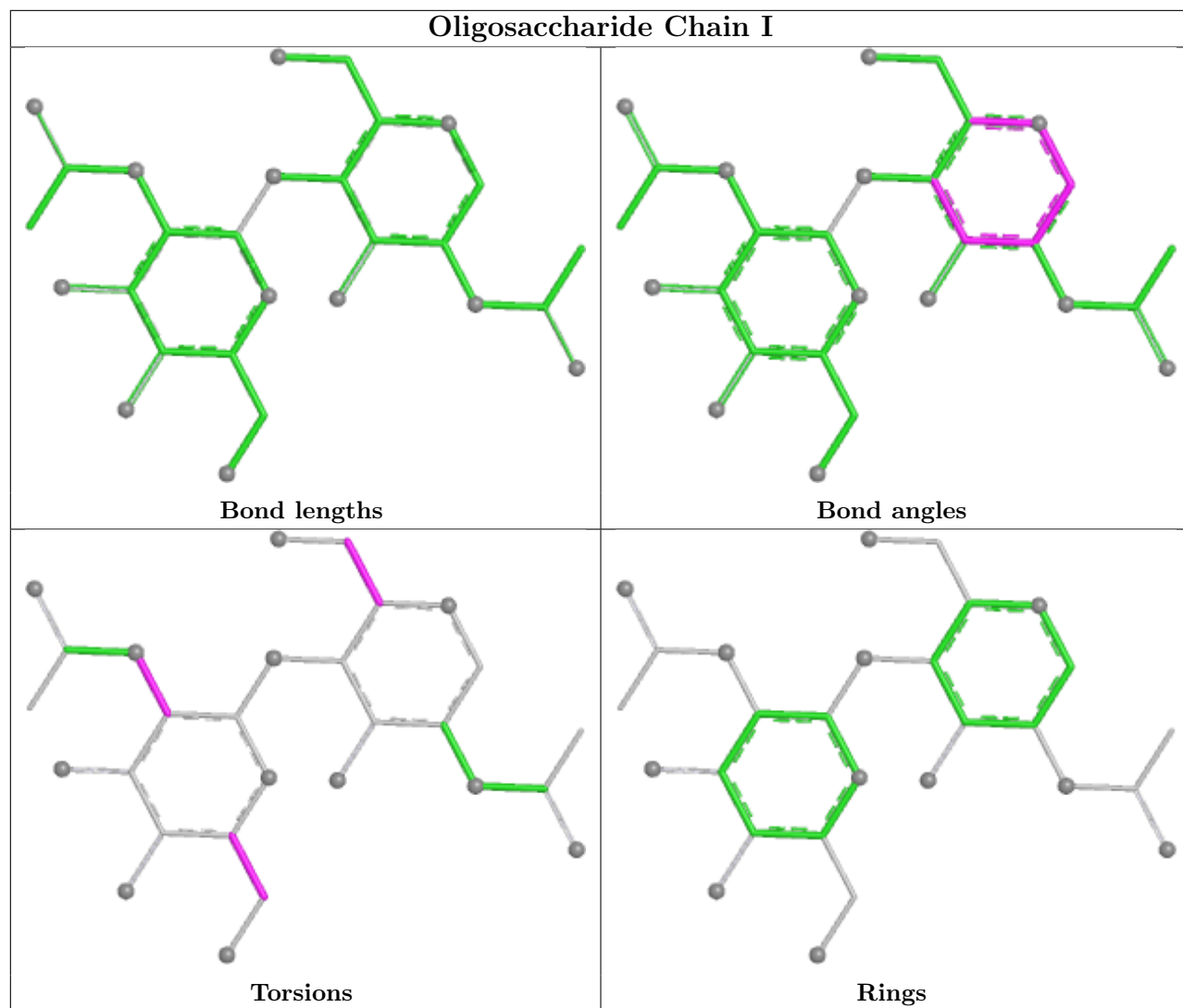
13 monomers are involved in 39 short contacts:

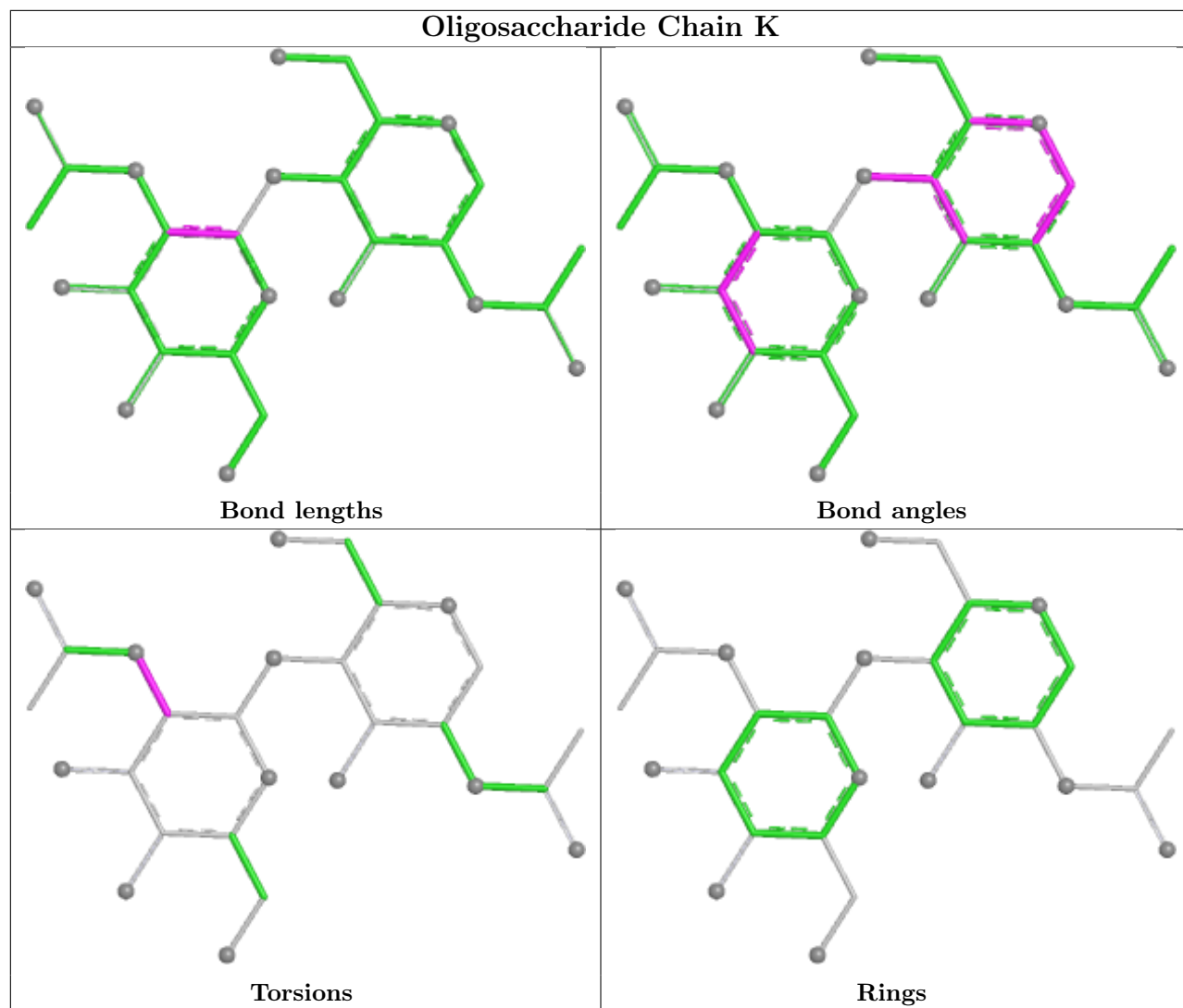
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	2	NAG	6	0
5	J	1	NAG	14	0
5	J	2	NAG	12	0
6	L	1	NAG	7	0
4	O	1	NAG	2	0
4	N	1	NAG	1	0
4	I	2	NAG	1	0
5	J	3	BMA	3	0
4	K	1	NAG	4	0
6	L	3	BMA	2	0
4	M	1	NAG	3	0
4	P	1	NAG	1	0
4	I	1	NAG	1	0

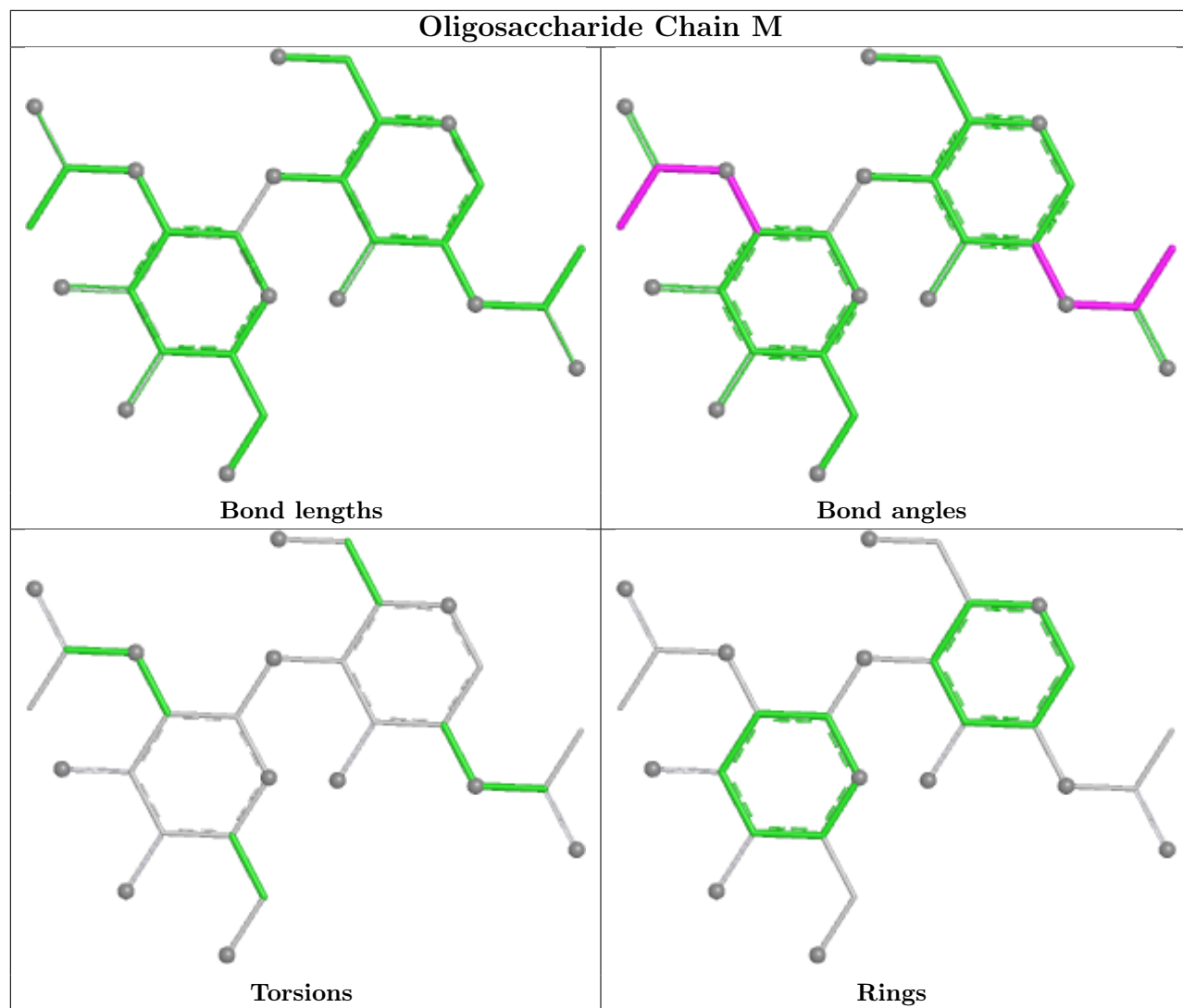
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

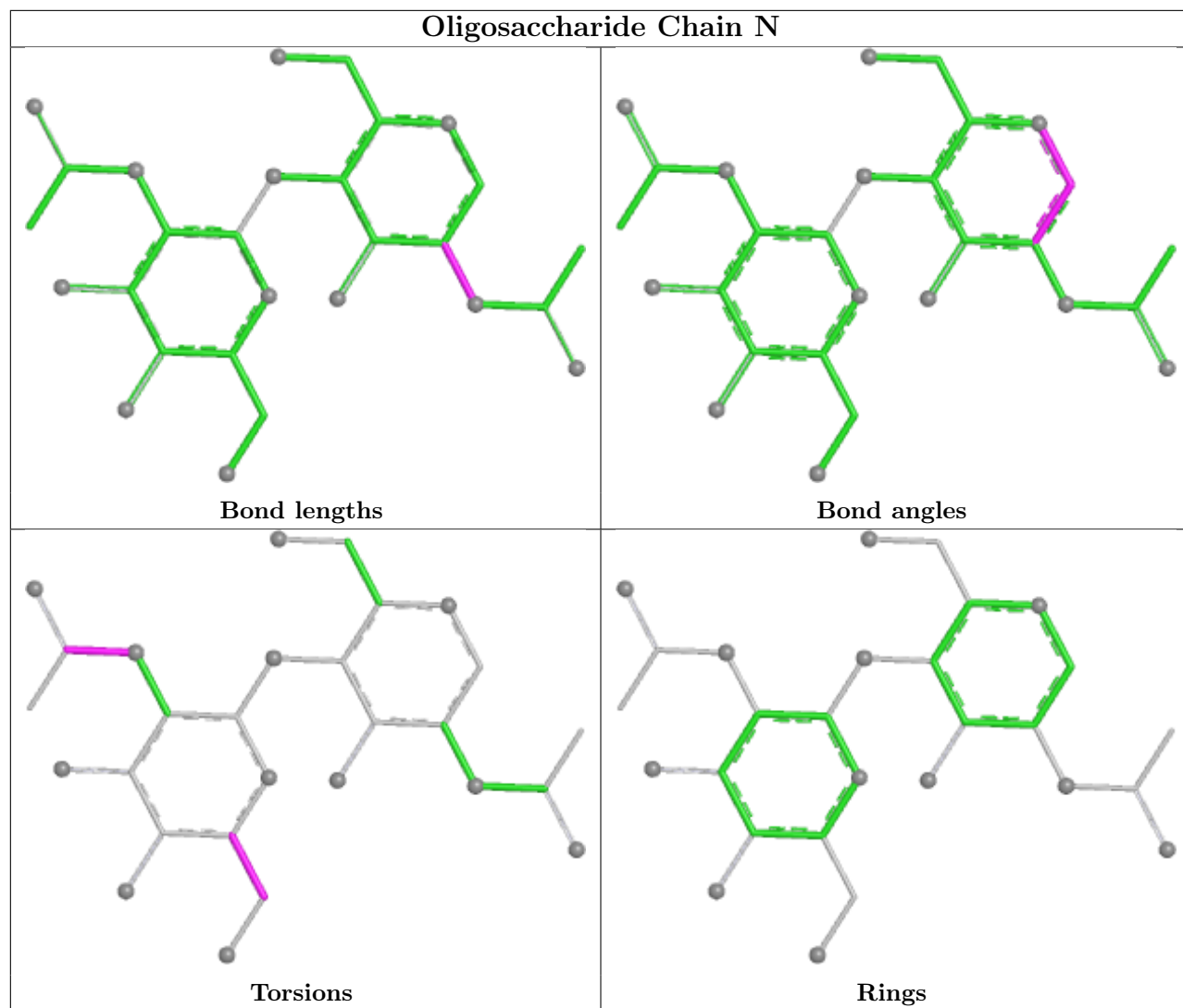
bond angles, torsion angles, and ring geometry for oligosaccharide.

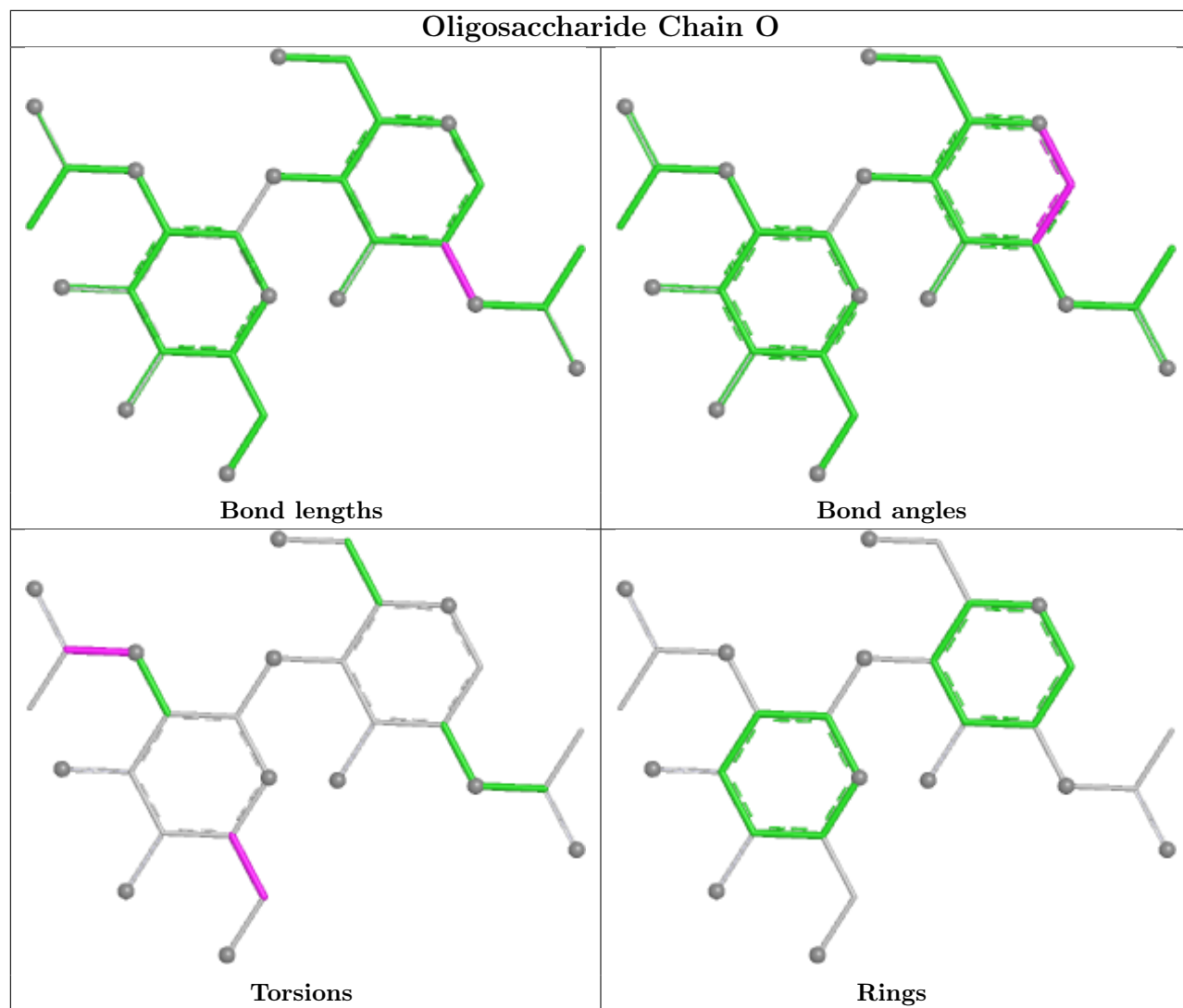


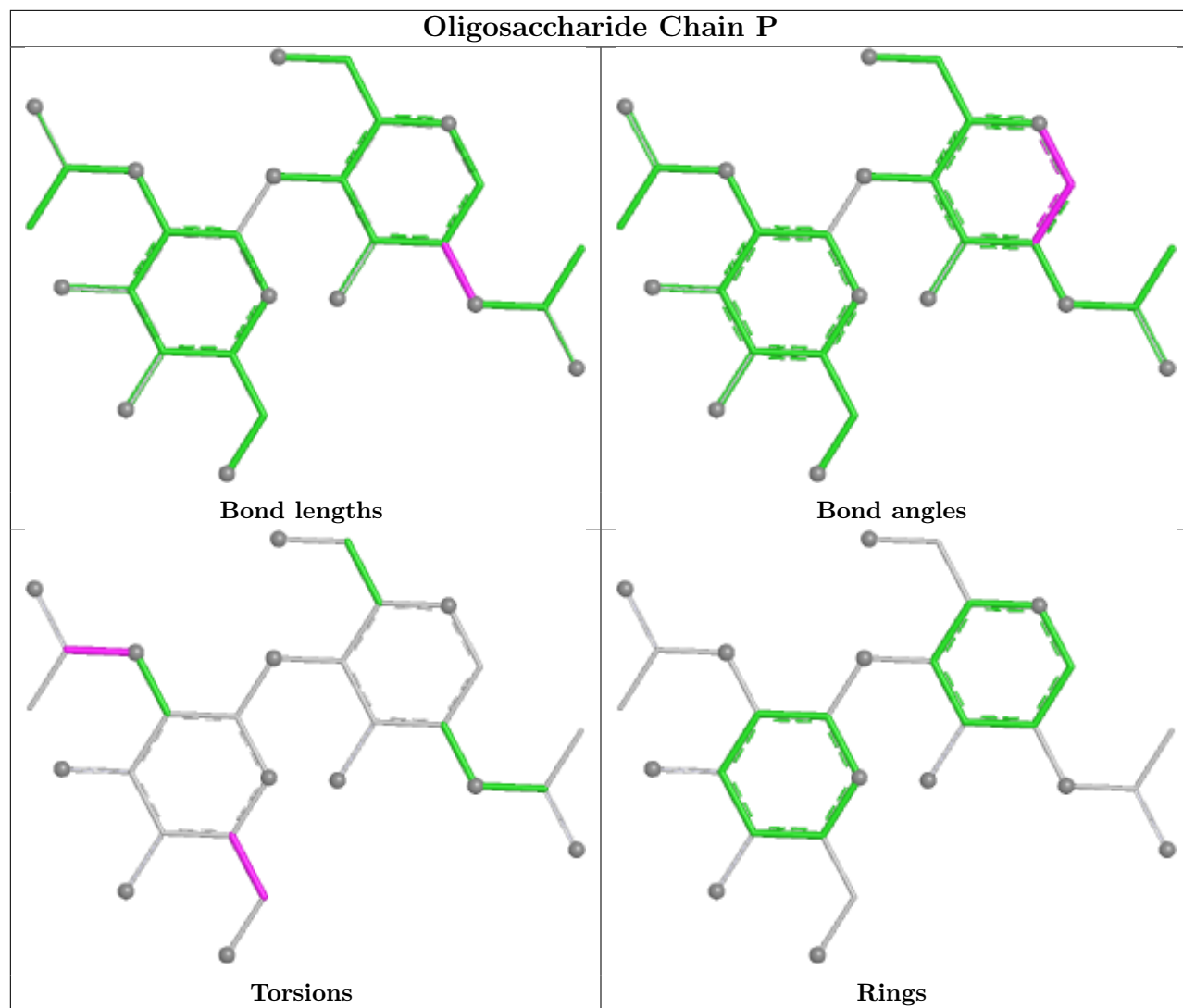


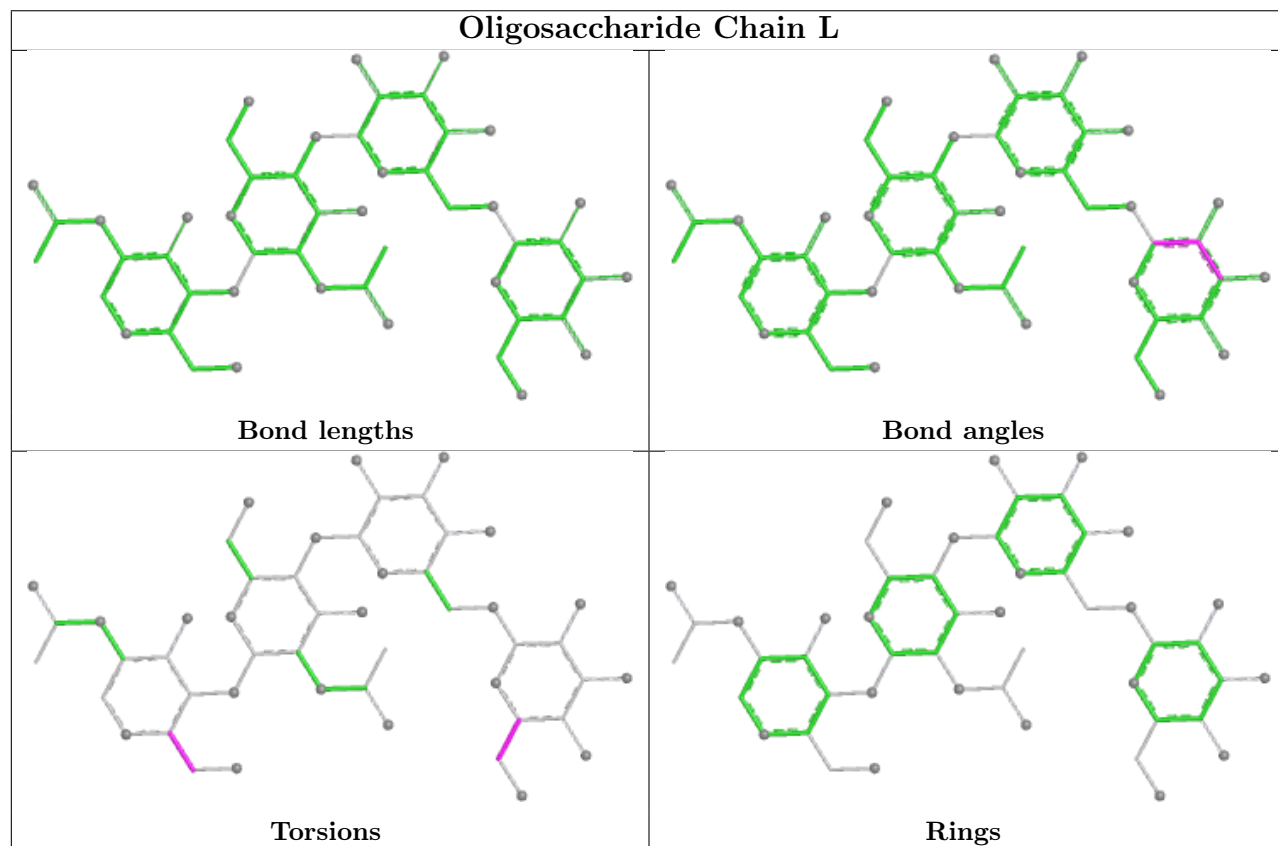
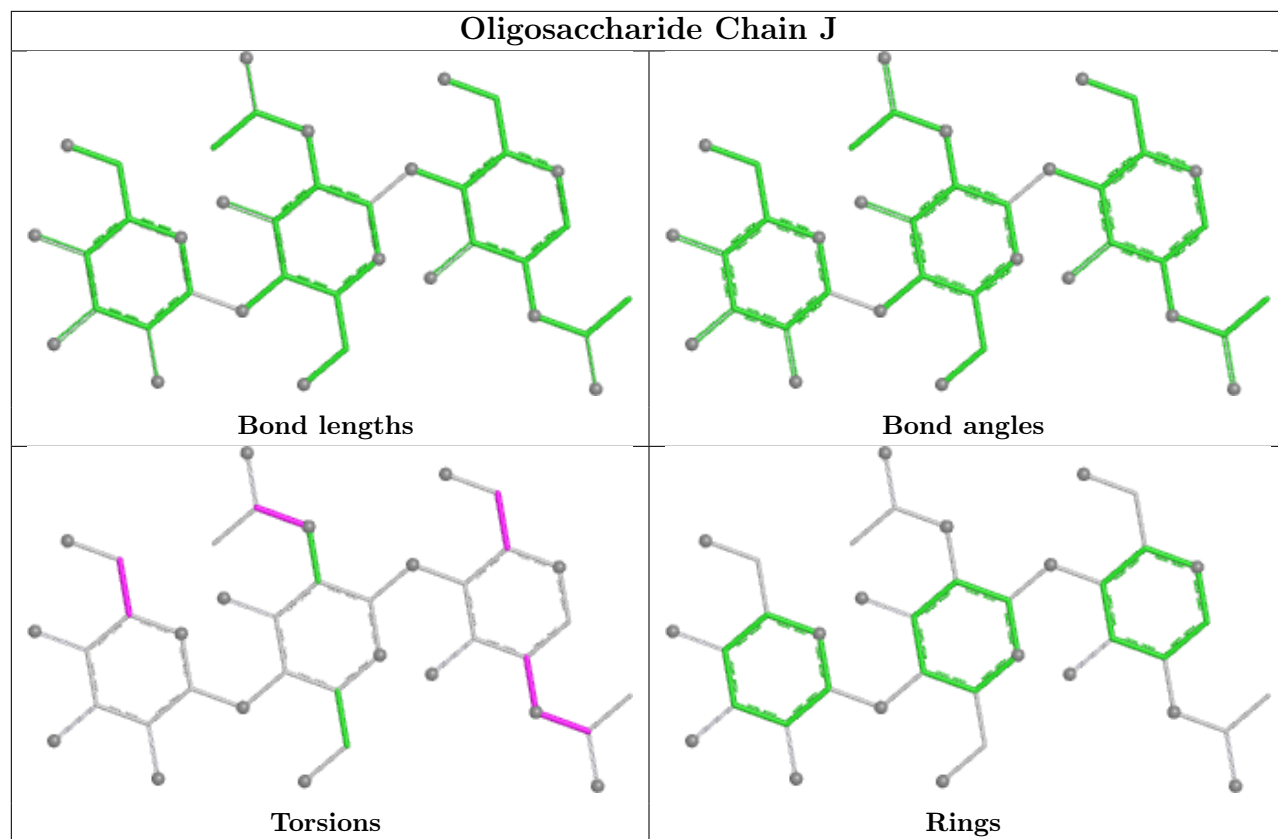












5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1317	1	14,14,15	0.29	0	17,19,21	0.56	0
7	NAG	A	1316	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
7	NAG	A	1321	-	14,14,15	0.30	0	17,19,21	0.56	0
7	NAG	A	1324	1	14,14,15	0.44	0	17,19,21	1.17	2 (11%)
7	NAG	A	1323	1	14,14,15	0.28	0	17,19,21	0.56	0
7	NAG	A	1303	1	14,14,15	0.30	0	17,19,21	0.55	0
7	NAG	A	1309	1	14,14,15	0.51	0	17,19,21	1.15	2 (11%)
7	NAG	A	1322	1	14,14,15	0.30	0	17,19,21	0.56	0
7	NAG	A	1320	1	14,14,15	0.30	0	17,19,21	0.56	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
7	NAG	A	1317	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1321	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1324	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1323	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	5/6/23/26	0/1/1/1
7	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1322	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1320	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1324	NAG	C8-C7-N2	2.32	119.97	116.12
7	A	1316	NAG	C8-C7-N2	2.30	119.94	116.12
7	A	1324	NAG	C2-N2-C7	-2.21	119.94	122.90
7	A	1316	NAG	C2-N2-C7	-2.17	120.00	122.90
7	A	1309	NAG	C1-C2-N2	-2.11	107.11	110.43

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1303	NAG	C8-C7-N2-C2
7	A	1303	NAG	O7-C7-N2-C2
7	A	1322	NAG	C8-C7-N2-C2
7	A	1322	NAG	O7-C7-N2-C2
7	A	1323	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1317	NAG	1	0
7	A	1324	NAG	2	0
7	A	1323	NAG	1	0
7	A	1303	NAG	1	0
7	A	1322	NAG	3	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.

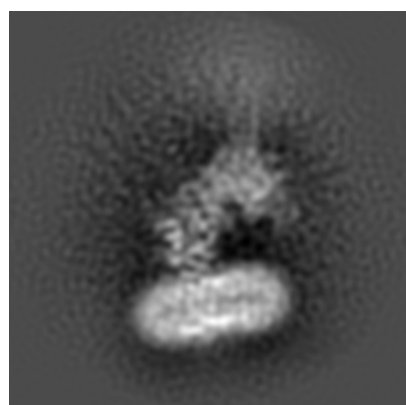
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8169. These allow visual inspection of the internal detail of the map and identification of artifacts.

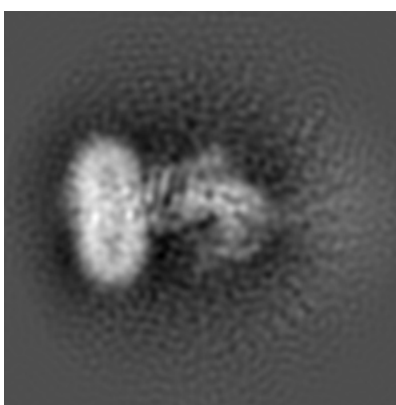
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

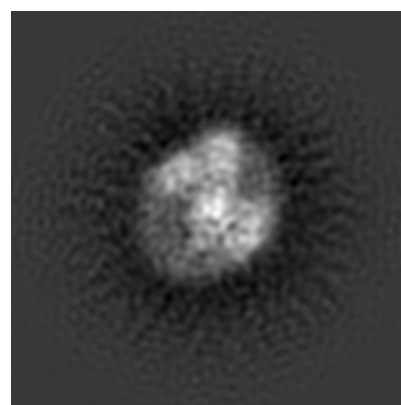
6.1.1 Primary map



X



Y

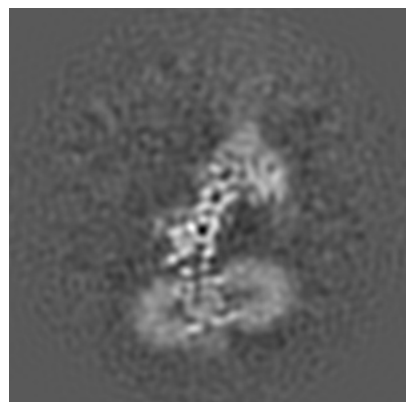


Z

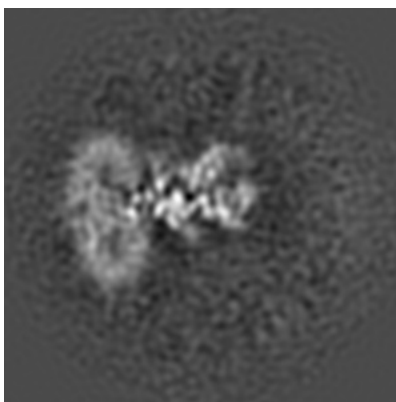
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

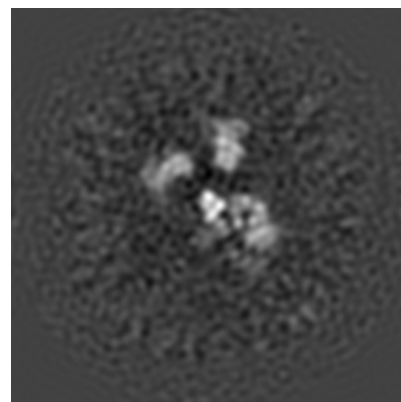
6.2.1 Primary map



X Index: 128



Y Index: 128

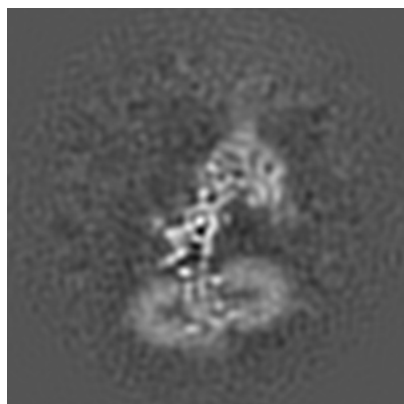


Z Index: 128

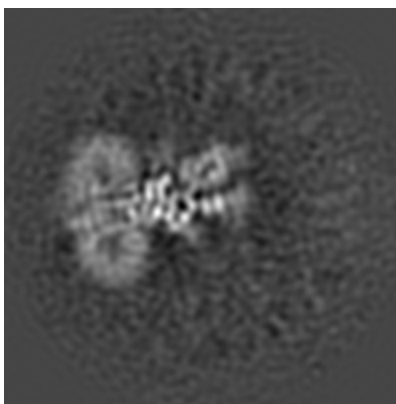
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

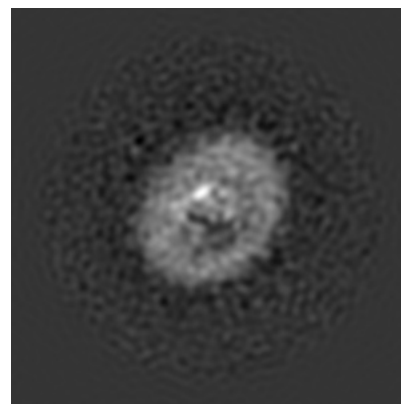
6.3.1 Primary map



X Index: 130



Y Index: 125

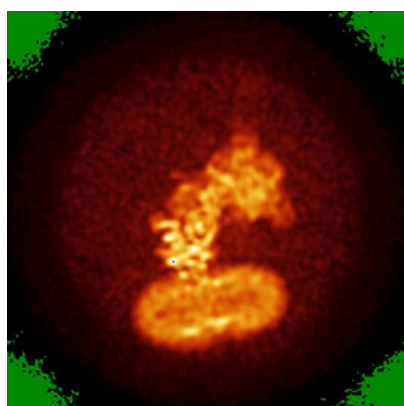


Z Index: 57

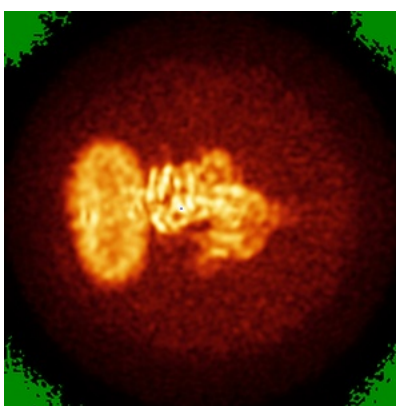
The images above show the largest variance slices of the map in three orthogonal directions.

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

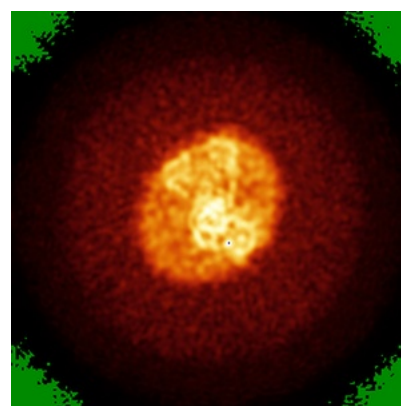
6.4.1 Primary map



X



Y

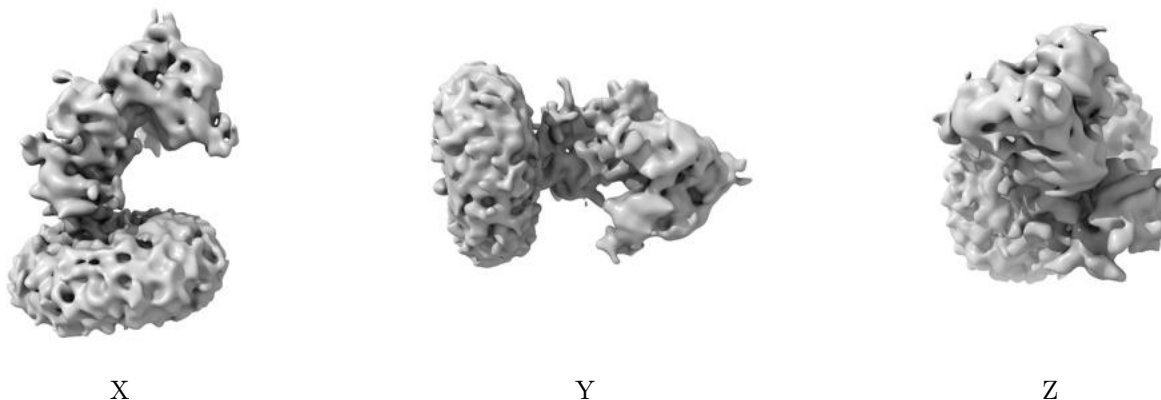


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

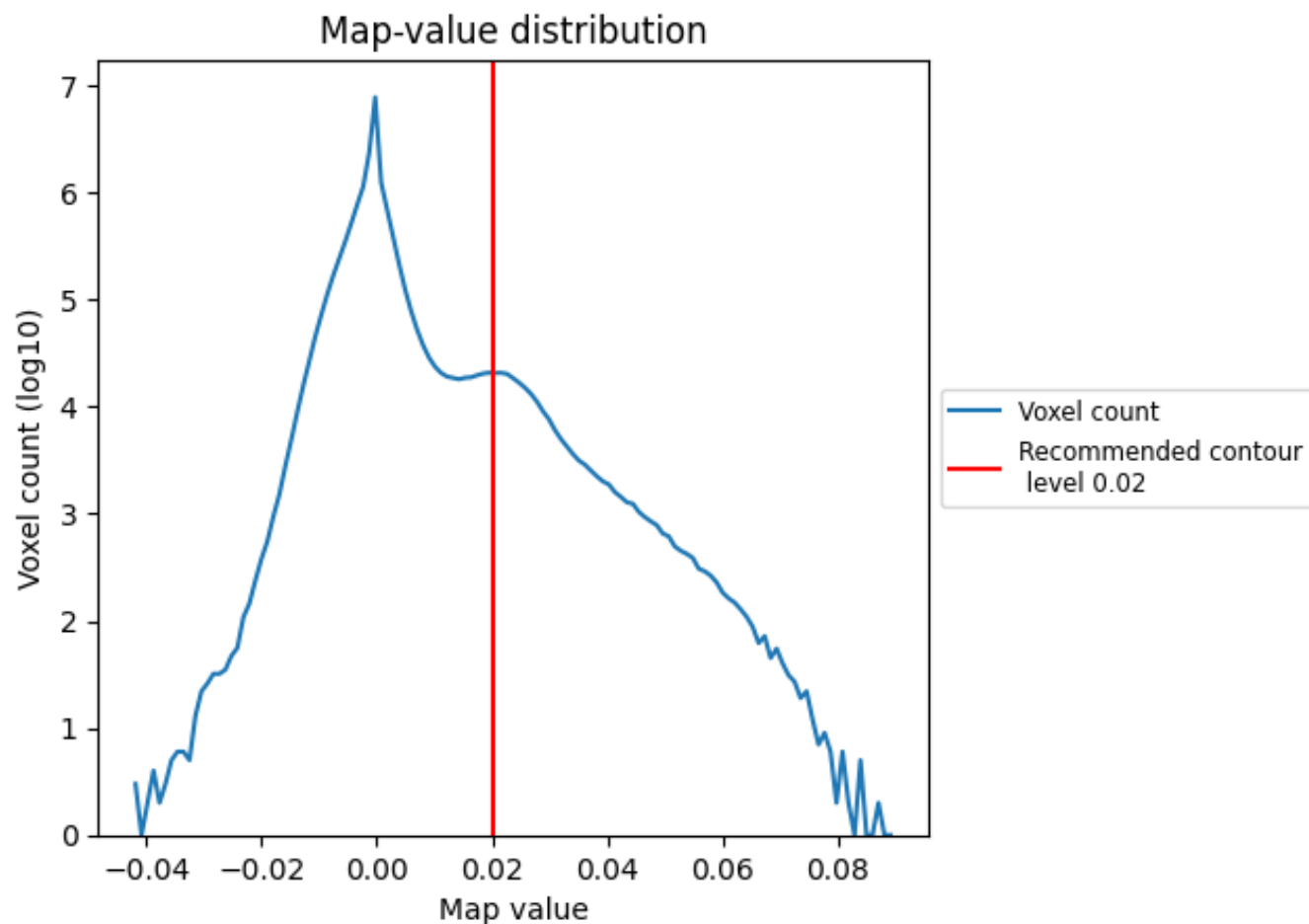
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

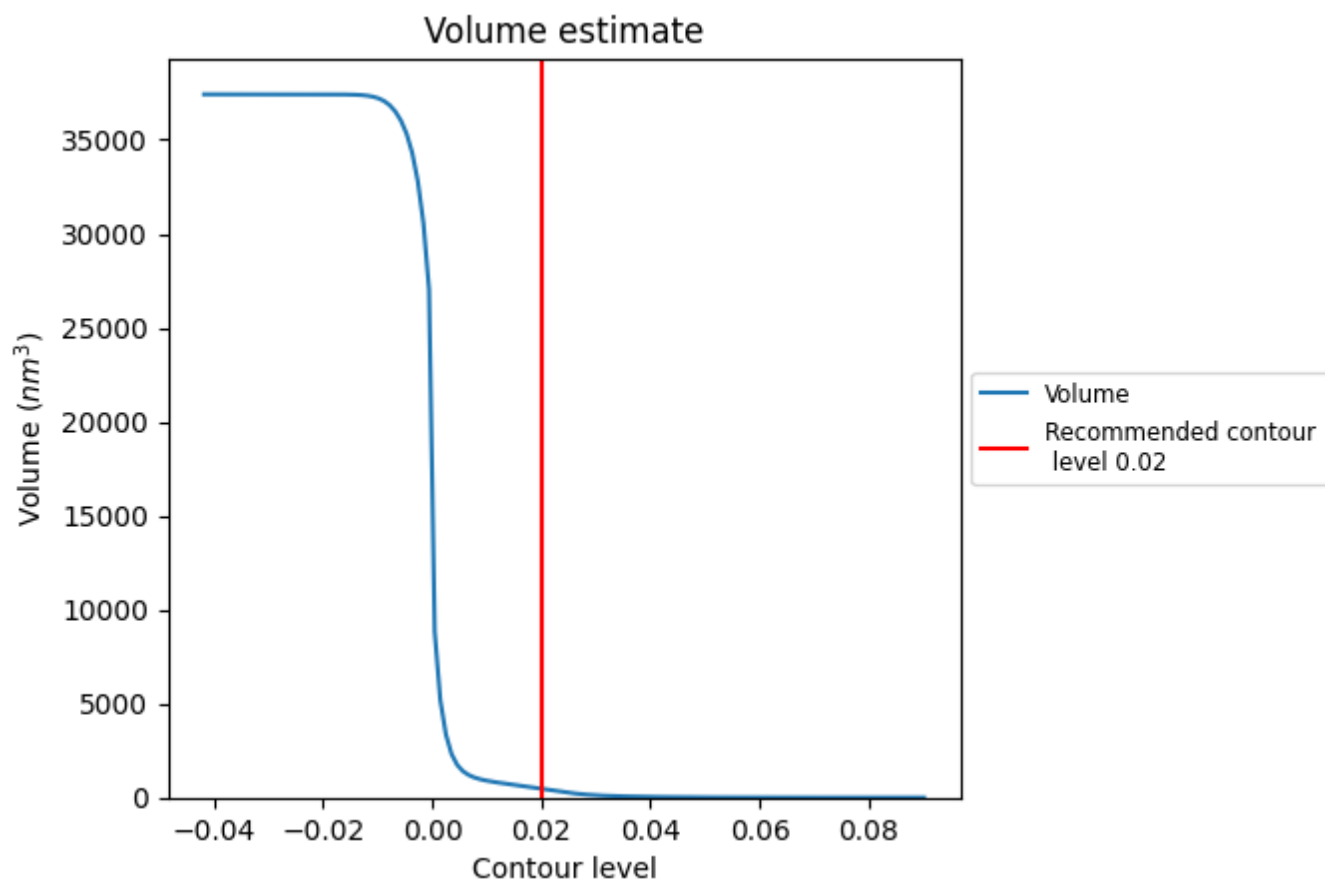
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

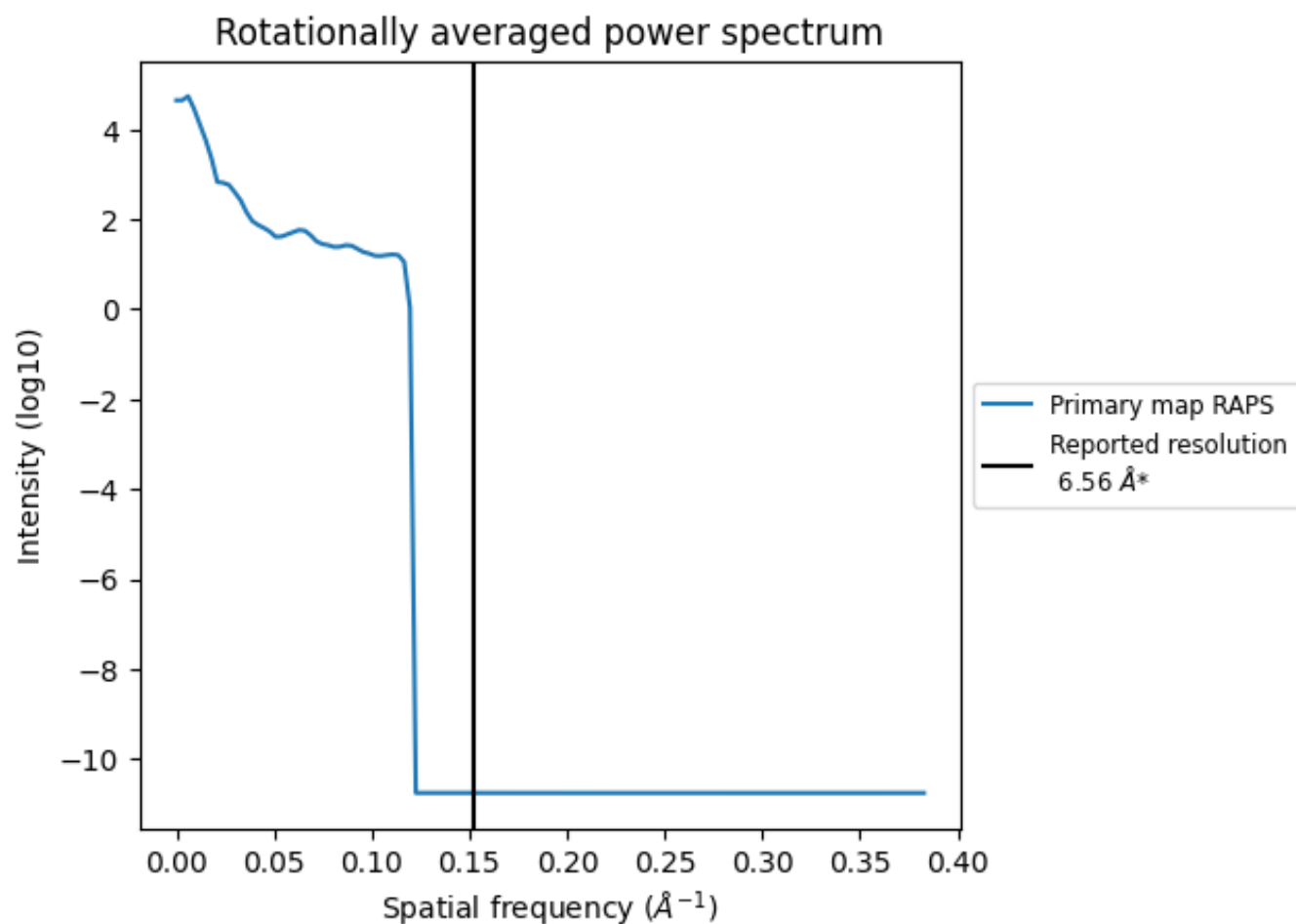
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 471 nm³; this corresponds to an approximate mass of 425 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 0.152 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

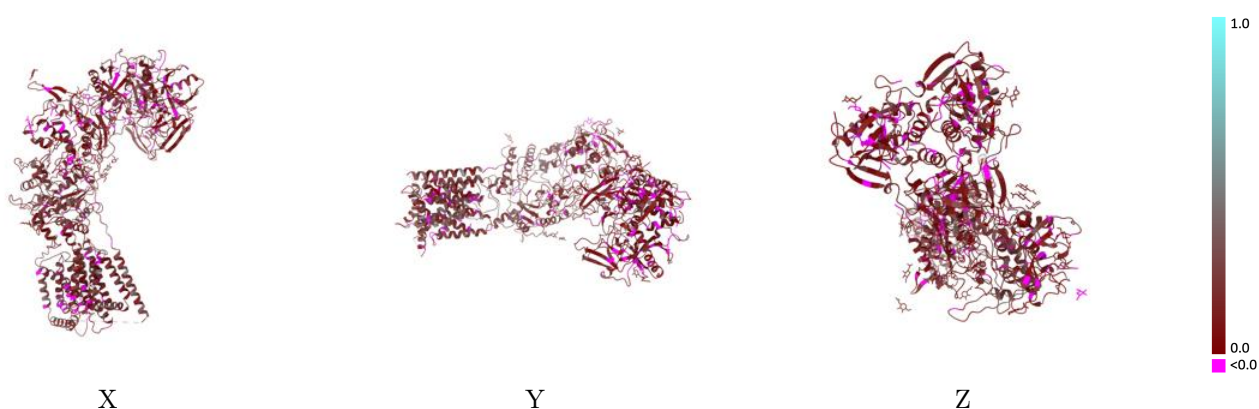
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8169 and PDB model 5JNX. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

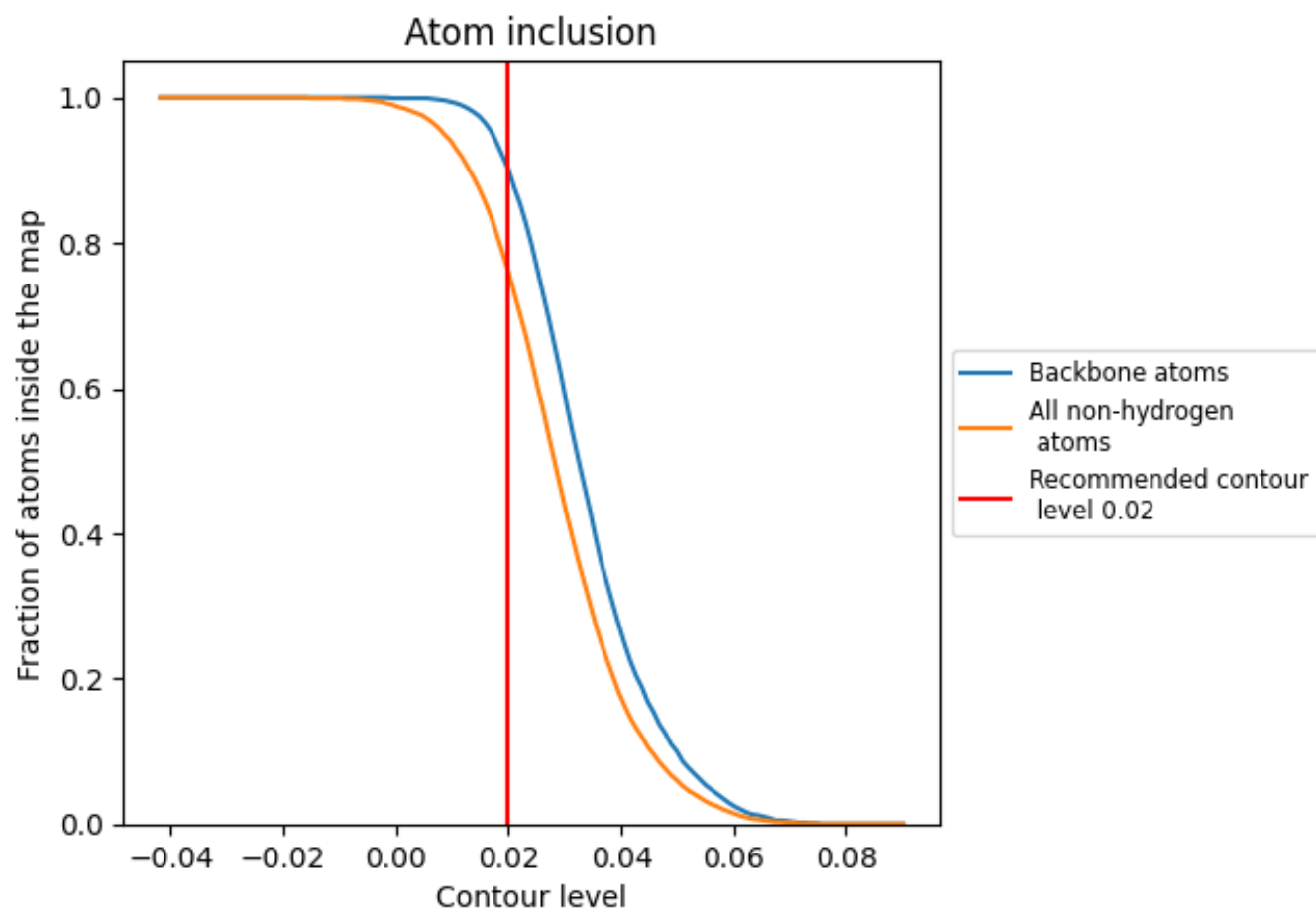


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.1400
A	 0.7690	 0.1550
B	 0.8210	 0.1610
C	 0.7490	 0.1050
D	 0.7890	 0.1200
E	 0.7250	 0.1120
F	 0.7780	 0.1470
G	 0.7530	 0.1110
H	 0.7900	 0.1460
I	 0.3210	 0.0630
J	 0.8460	 0.1830
K	 0.8210	 0.2580
L	 0.7800	 0.2320
M	 0.0710	 0.1200
N	 0.2140	 0.0730
O	 0.1070	 0.0200
P	 0.7140	 0.1440

